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NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	AUG 10	Time limit for inactive STN sessions doubles to 40 minutes
NEWS	3	AUG 18	COMPENDEX indexing changed for the Corporate Source (CS) field
NEWS	4	AUG 24	ENCOMPLIT/ENCOMPLIT2 reloaded and enhanced
NEWS	5	AUG 24	CA/CAplus enhanced with legal status information for U.S. patents
NEWS	6	SEP 09	50 Millionth Unique Chemical Substance Recorded in CAS REGISTRY
NEWS	7	SEP 11	WPIDS, WPINDEX, and WPIX now include Japanese FTERM thesaurus
NEWS	8	OCT 21	Derwent World Patents Index Coverage of Indian and Taiwanese Content Expanded
NEWS	9	OCT 21	Derwent World Patents Index enhanced with human translated claims for Chinese Applications and Utility Models
NEWS	10	NOV 23	Addition of SCAN format to selected STN databases
NEWS	11	NOV 23	Annual Reload of IFI Databases
NEWS	12	DEC 01	FRFULL Content and Search Enhancements
NEWS	13	DEC 01	DGENE, USGENE, and PCTGEN: new percent identity feature for sorting BLAST answer sets
NEWS	14	DEC 02	Derwent World Patent Index: Japanese FI-TERM thesaurus added
NEWS	15	DEC 02	PCTGEN enhanced with patent family and legal status display data from INPADOCDB
NEWS	16	DEC 02	USGENE: Enhanced coverage of bibliographic and sequence information
NEWS	17	DEC 21	New Indicator Identifies Multiple Basic Patent Records Containing Equivalent Chemical Indexing in CA/CAplus
NEWS	18	JAN 12	Match STN Content and Features to Your Information Needs, Quickly and Conveniently
NEWS	19	JAN 25	Annual Reload of MEDLINE database

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

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FILE 'HOME' ENTERED AT 21:45:56 ON 28 JAN 2010

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.22	0.22

FILE 'REGISTRY' ENTERED AT 21:46:12 ON 28 JAN 2010
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 27 JAN 2010 HIGHEST RN 1203797-79-8
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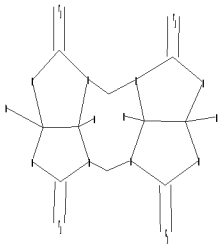
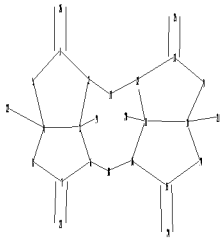
http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10598861\Struc 3.str





chain nodes :
19 20 21 22 23 24 25 26
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
chain bonds :
1-26 3-19 4-22 7-23 10-21 11-20 13-25 15-24
ring bonds :
1-2 1-5 2-3 2-17 3-4 3-6 4-5 4-8 6-7 6-18 7-8 9-10 9-13 10-11 10-14
11-12 11-16 12-13 12-17 14-15 15-16 16-18
exact/norm bonds :
1-2 1-5 1-26 2-3 2-17 3-4 3-6 3-19 4-5 4-8 4-22 6-7 6-18 7-8 7-23
9-10 9-13 10-11 10-14 11-12 11-16 12-13 12-17 13-25 14-15 15-16 15-24
16-18
exact bonds :
10-21 11-20

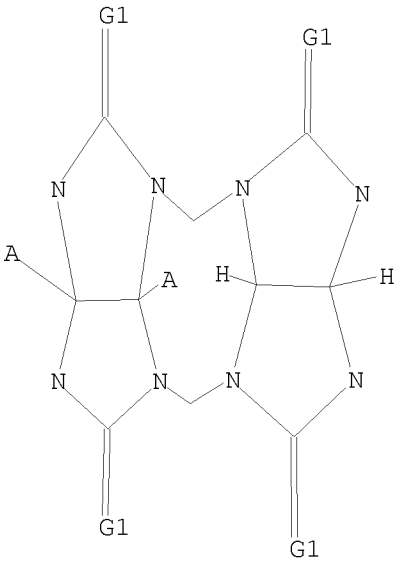
G1:O,S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS

10598861b.trn

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> l1
SAMPLE SEARCH INITIATED 21:46:30 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 105 TO ITERATE

100.0% PROCESSED 105 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1486 TO 2714
PROJECTED ANSWERS: 3 TO 163

L2 3 SEA SSS SAM L1

=> l1 full
FULL SEARCH INITIATED 21:46:33 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1880 TO ITERATE

100.0% PROCESSED 1880 ITERATIONS 56 ANSWERS
SEARCH TIME: 00.00.01

L3 56 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 191.54 191.76

FILE 'CAPLUS' ENTERED AT 21:46:36 ON 28 JAN 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 28 Jan 2010 VOL 152 ISS 5
FILE LAST UPDATED: 27 Jan 2010 (20100127/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2009

CAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

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http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l3
L4 30 L3

=> d ibib abs hitstr 1-30

L4 ANSWER 1 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:1211987 CAPLUS
DOCUMENT NUMBER: 151:508271
TITLE: Exclusion complexes of the HCl salts of benzidine and bis(4-aminophenyl) methane with two methyl-substituted cucurbiturils
AUTHOR(S): Yan, Ying; Xue, Sai-Feng; Cong, Hang; Zhang, Jian-Xing; Zhang, Yun-Qian; Zhu, Qian-Jiang; Tao, Zhu
CORPORATE SOURCE: Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: New Journal of Chemistry (2009), 33(10), 2136-2143
CODEN: NJCHE5; ISSN: 1144-0546
PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal
LANGUAGE: English

AB The interaction between two partially methyl-substituted cucurbiturils, a sym-tetramethyl-substituted cucurbit[6]uril (TMeQ[6]) and a meta-hexamethyl-substituted cucurbituril (m-HMeQ[6]), with the hydrochloride salt of benzidine (g1·HCl) and the analog bis(4-aminophenyl) methane (g2·HCl) was investigated by single crystal X-ray diffraction determination, 1H NMR spectroscopy, electronic absorption spectroscopy and fluorescence spectroscopy. Single crystal X-ray diffraction determination showed the two guest compds. were excluded at the portals of the partial methyl-substituted cucurbiturils in the solid state. The 1H NMR spectroscopic anal. in aqueous solution supported the crystallog. results in which an excluding or portal interaction occurs between the host and guest. Aqueous absorption spectrophotometric and fluorescence spectroscopic anal. defined the stability of the host-guest exclusion complex at pH 5.6 with a host : guest ratio of 1 : 1, which forms quant. as .apprx.105 L mol-1 for the TMeQ[6]-g1 system. The host : guest ratio of 2 : 1 forms quant. as .apprx.1010 L2 mol-2 for the m-HMeQ[6]-g2 system. The exptl. results are in good agreement with HF and B3LYP computational approaches with a moderate-sized basis set.

IT 1193130-36-7 1193130-39-0
RL: PRP (Properties)
(exclusion complexes of the HCl salts of benzidine and bisaminophenyl methane with two methylsubstituted cucurbiturils)

RN 1193130-36-7 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

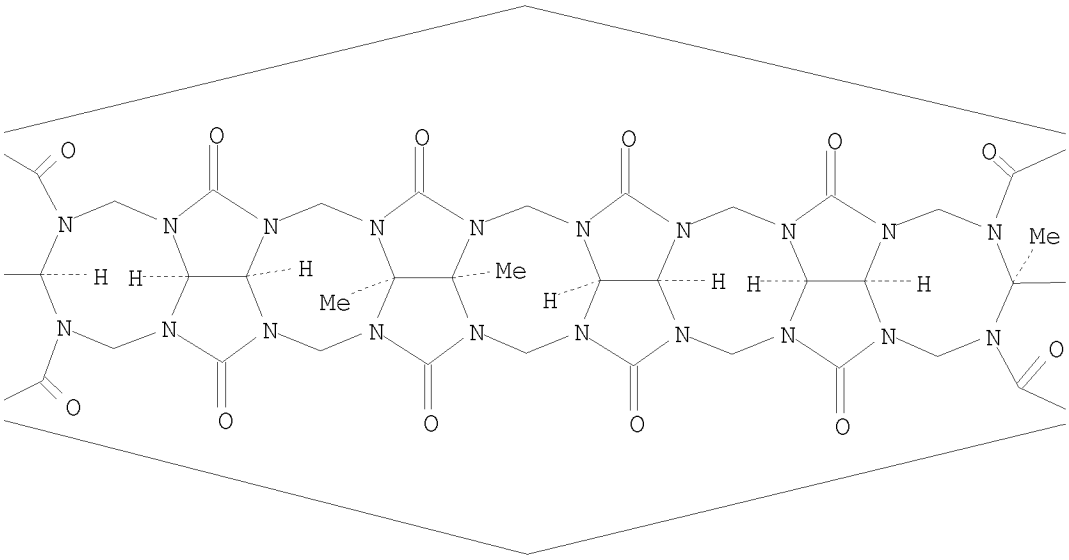
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

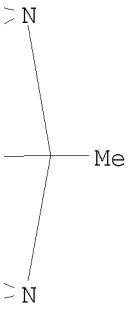
Relative stereochemistry.

PAGE 1-A

PAGE 1-B

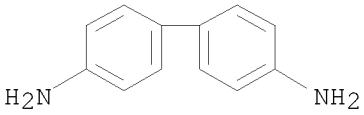


PAGE 1-C



CM 2

CRN 92-87-5
CMF C12 H12 N2



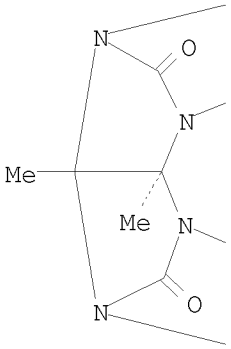
RN 1193130-39-0 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

CM 1

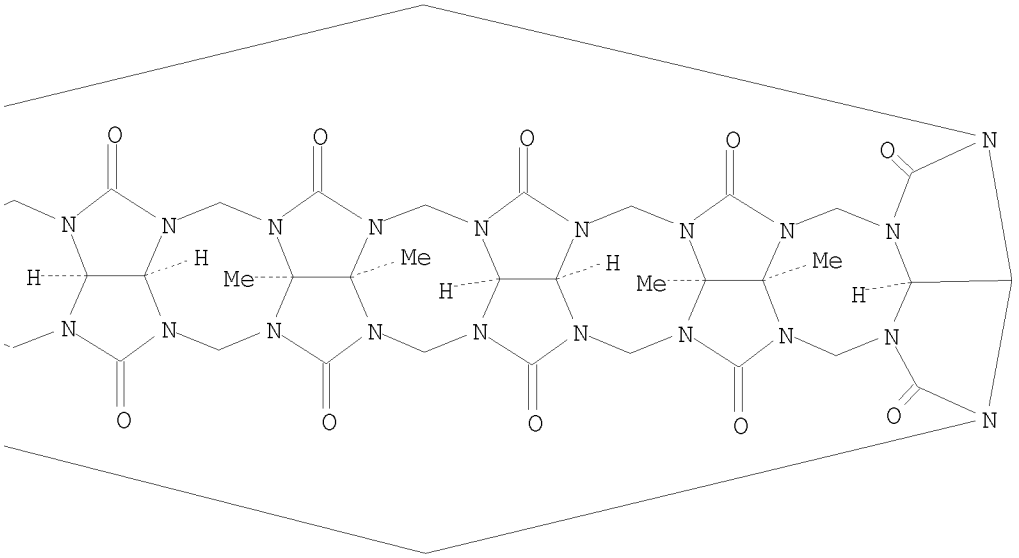
CRN 640732-36-1
CMF C42 H48 N24 O12

Relative stereochemistry.

PAGE 1-A

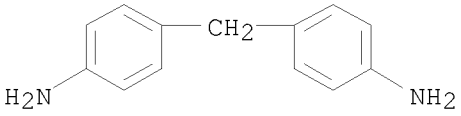


PAGE 1-B



CM 2

CRN 101-77-9
CMF C13 H14 N2



REFERENCE COUNT: 78 THERE ARE 78 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:1052686 CAPLUS
TITLE: Formation of host-guest complexes of 3-(aminomethyl)pyridine HCl salt and tetramethylcucurbit[6]uril
AUTHOR(S): Zhao, Fang Fang; Cong, Hang; Tao, Zhu; Xue, Sai Feng; Zhu, Qian Jiang
CORPORATE SOURCE: Institute of Applied Chemistry, Guizhou University, Guiyang, Peop. Rep. China
SOURCE: Asian Journal of Chemistry (2009), 21(7), 5737-5740
CODEN: AJCHEW; ISSN: 0970-7077
PUBLISHER: Asian Journal of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The structure of complex of 3-(aminomethyl)pyridine hydrochloride (AMPY+, guest) and sym. tetra-Me substituted cucurbit[6]uril (TMeQ[6], host) has been studied by single crystal x-ray diffraction. Association consts. of 9.51 + 105 L/methanol for 1:1 complexes were determined by UV-vis spectra titration
IT 1203675-46-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure; formation and crystal structure of host-guest complexes of 3-(aminomethyl)pyridine and tetramethylcucurbit[6]uril)
RN 1203675-46-0 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

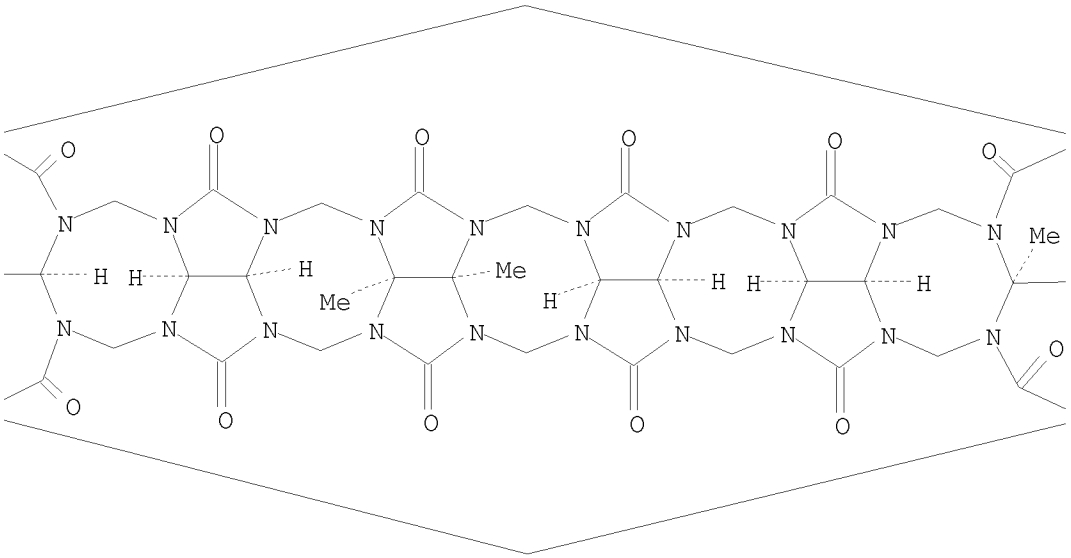
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

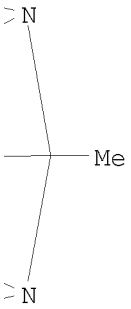
Relative stereochemistry.

PAGE 1-A

PAGE 1-B

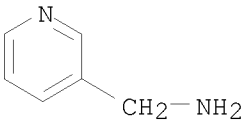


PAGE 1-C



CM 2

CRN 84359-15-9
CMF C6 H8 N2 . Cl H



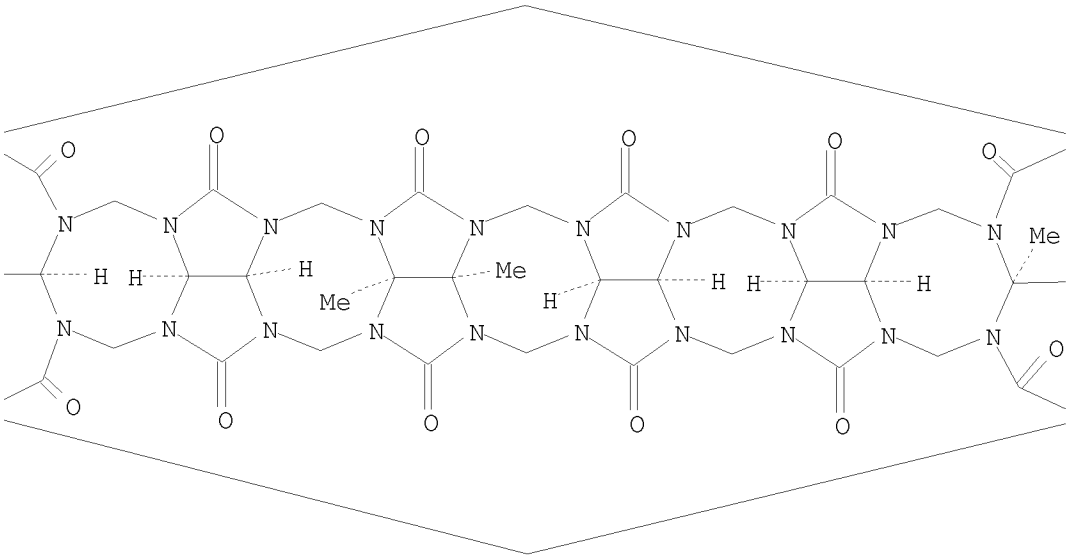
● HCl

IT 848440-56-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(formation and crystal structure of host-guest complexes of 3-(aminomethyl)pyridine and tetramethylcucurbit[6]uril)
RN 848440-56-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

PAGE 1-B



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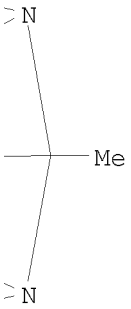
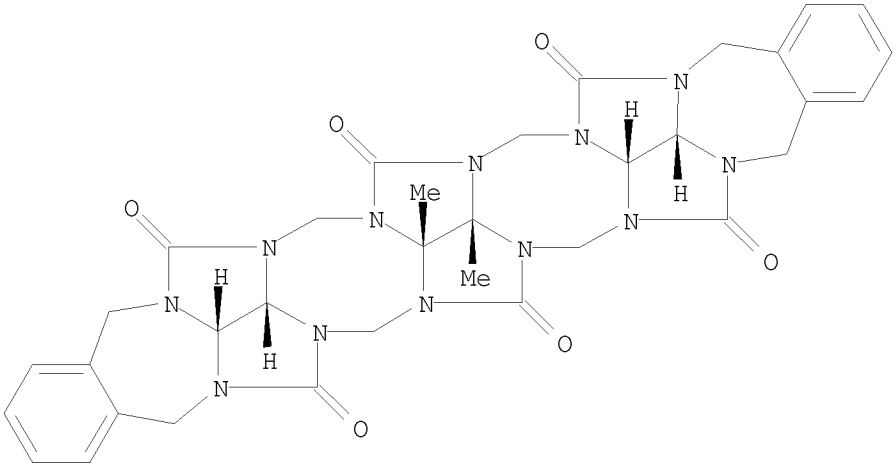


REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:1046044 CAPLUS
DOCUMENT NUMBER: 151:358134
TITLE: Glycoluril Trimers: Selective Synthesis and Supramolecular Properties
AUTHOR(S): Stancl, Marek; Hodan, Martin; Sindelar, Vladimir
CORPORATE SOURCE: Department of Chemistry, Masaryk University, Brno, 611 37, Czech Rep.
SOURCE: Organic Letters (2009), 11(18), 4184-4187
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The first selective synthesis of glycoluril trimers is described. Trimers framed by o-xylylene walls represent new supramol. hosts which are able to encapsulate bispyridinium ethylene and methylviologen guests in the solid state and aqueous solution
IT 1186661-73-3P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(crystal structure; selective synthesis and supramol. properties of glycoluril trimers)
RN 1186661-73-3 CAPLUS
CN 6H,7H,8H,9H,10H,17H,18H,19H,20H,21H-5a,6a,7a,8a,9a,10a,16a,17a,18a,19a,20a,21a-Dodecaazabisbenzo[5'',6'']cyclohepta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-6,8,10,17,19,21-hexone, 5,11,16,17b,17c,19b,19c,21b,21c,22-decahydro-19b,19c-dimethyl-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

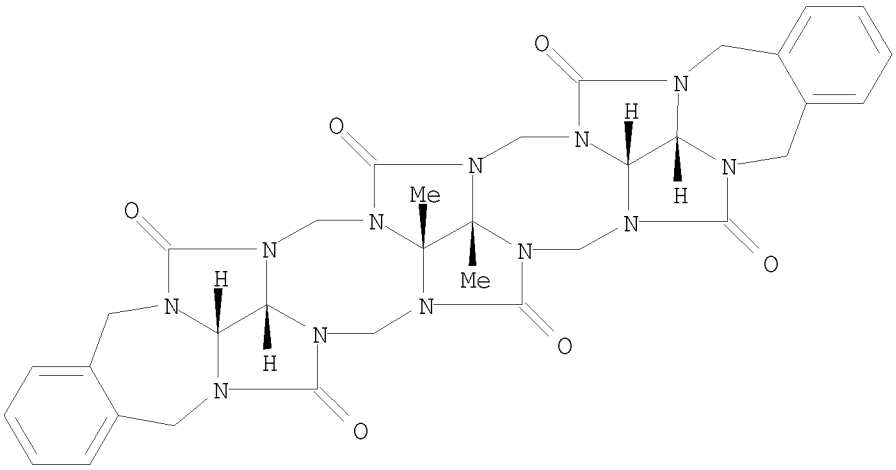


IT 1186661-78-8P 1186661-82-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; selective synthesis and supramol. properties of glycoluril trimers)
RN 1186661-78-8 CAPLUS
CN Pyridinium, 4,4'-(1E)-1,2-ethenediylbis[1-methyl-, compd. with stereoisomer of 5,11,16,17b,17c,19b,19c,21b,21c,22-decahydro-19b,19c-dimethyl-6H,7H,8H,9H,10H,17H,18H,19H,20H,21H-5a,6a,7a,8a,9a,10a,16a,17a,18a,19a,20a,21a-dodecaazabisbenzo[5'',6'']cyclohepta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-6,8,10,17,19,21-hexone (1:2) (CA INDEX NAME)

CM 1

CRN 1186661-73-3
CMF C34 H34 N12 O6

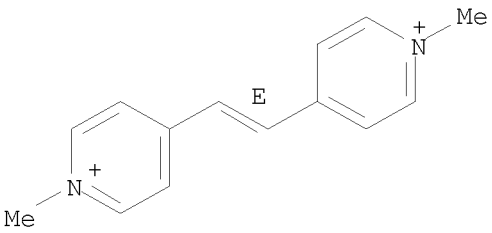
Relative stereochemistry.



CM 2

CRN 46740-72-1
CMF C14 H16 N2

Double bond geometry as shown.

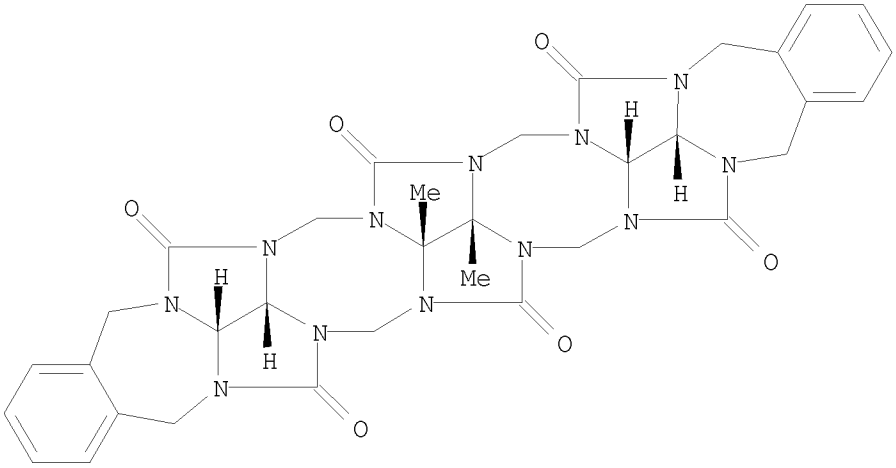


RN 1186661-82-4 CAPLUS
CN 4,4'-Bipyridinium, 1,1'-dimethyl-, compd. with stereoisomer of 5,11,16,17b,17c,19b,19c,21b,21c,22-decahydro-19b,19c-dimethyl-6H,7H,8H,9H,10H,17H,18H,19H,20H,21H-5a,6a,7a,8a,9a,10a,16a,17a,18a,19a,20a,21a-dodecaazabisbenzo[5'',6'']cyclohepta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-6,8,10,17,19,21-hexone (1:1) (CA INDEX NAME)

CM 1

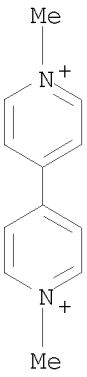
CRN 1186661-73-3
CMF C34 H34 N12 O6

Relative stereochemistry.



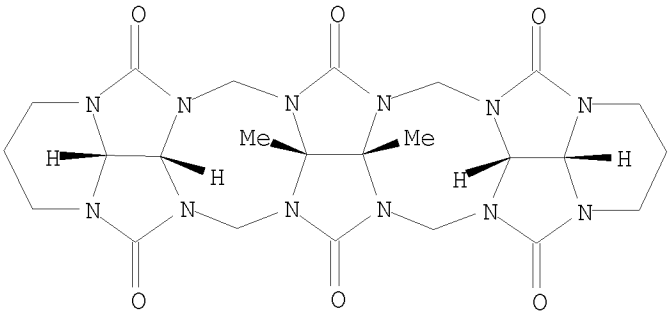
CM 2

CRN 4685-14-7
CMF C12 H14 N2



IT 1186661-77-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(selective synthesis and supramol. properties of glycoluril trimers)
RN 1186661-77-7 CAPLUS
CN 1H,4H,5H,6H,7H,8H,9H,12H,13H,14H,15H,16H-3a,4a,5a,6a,7a,8a,11a,12a,13a,14a,15a,16a-Dodecaazabisbenzo[3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-4,6,8,12,14,16-hexone, decahydro-14b,14c-dimethyl-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:934355 CAPLUS
DOCUMENT NUMBER: 151:414996
TITLE: Crystal structures of four host-guest inclusion complexes of α,α',δ,δ'-tetramethylcucurbit[6]uril and cucurbit[8]uril with some L-amino acids
AUTHOR(S): Yi, Jun-Ming; Zhang, Yun-Qian; Cong, Hang; Xue, Sai-Feng; Tao, Zhu
CORPORATE SOURCE: Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Journal of Molecular Structure (2009), 933(1-3), 112-117
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Four crystal structures of inclusion complexes of amino acid and cucurbit[n]uril were synthesized and characterized by x-ray diffractions. The used 4 amino acids are L-glutamic acid (L-Glu), L-tyrosine (L-Tyr), L-histidine (L-His), L-leucine (L-Leu), and the hosts are α,α',δ,δ'-tetramethylcucurbit[6]uril (TMeQ[6]), the normal cucurbit[8]uril (Q[8]). The corresponding compds. based on the inclusion complexes of amino acid and cucurbit[n]uril have stoichiometry of {L-Glu@TMeQ[6]}+.cntdot.Cl-.cntdot.13H2O (1), {(L-Tyr)2@Q[8]}.cntdot.27H2O (2), {(L-His)2@Q[8]}.cntdot.19H2O (3), and {(L-Leu)2@Q[8]}2+.cntdot.2Cl-.cntdot.32H2O (4). The crystal structure of 1 reveals that a L-Glu mol. is captured by a host TMeQ[6] with a 1:1 host:guest ratio. The crystal structures of 2, 3, and 4 show that all 3 inclusion complexes of L-Tyr@Q[8], L-His@Q[8] and L-Leu@Q[8] are in 1:2 host:guest ratio. The host Q[8] can include not only 2 aromatic moieties from 2 same guests (such as in the cases of 2 and 3) but also 2 alkyl chains of 2 L-Leu mols. (the case of 4). Crystallog. data are given.
IT 1189113-40-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal and mol. structure of)
RN 1189113-40-3 CAPLUS
CN L-Glutamic acid, compd. with stereoisomer of dodecahydro-2a,21b,21c,26b-tetramethyl-1H,4H,14H,17H-2,16:3,15-dimethano-

5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24
a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2''
,3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-
g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone, hydrochloride, hydrate
(1:1:1:13) (CA INDEX NAME)

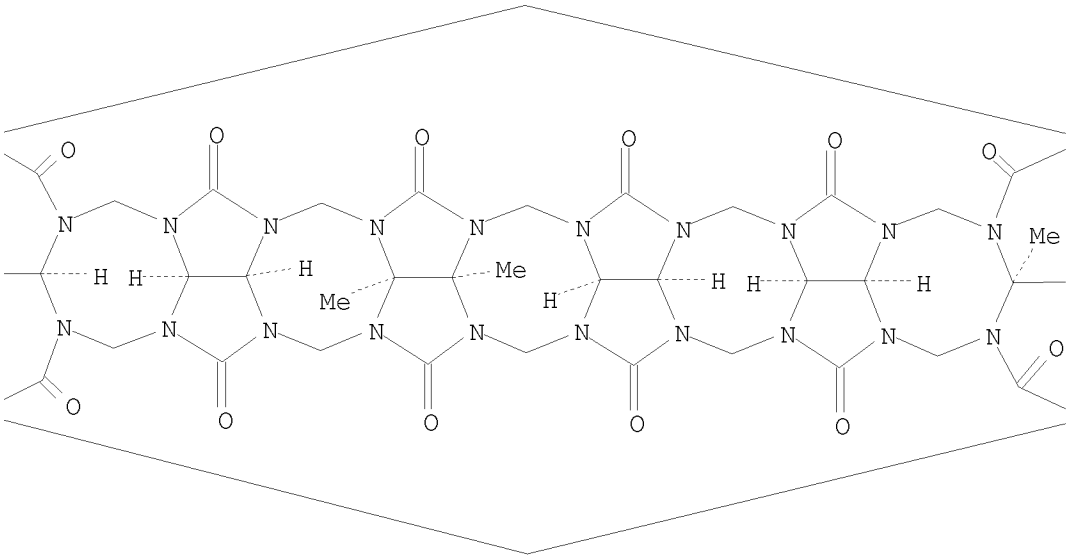
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

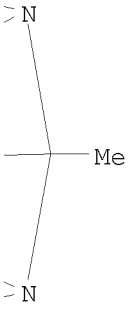
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



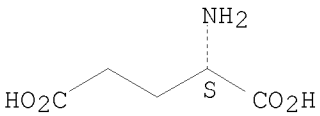
PAGE 1-C



CM 2

CRN 56-86-0
CMF C5 H9 N O4

Absolute stereochemistry.

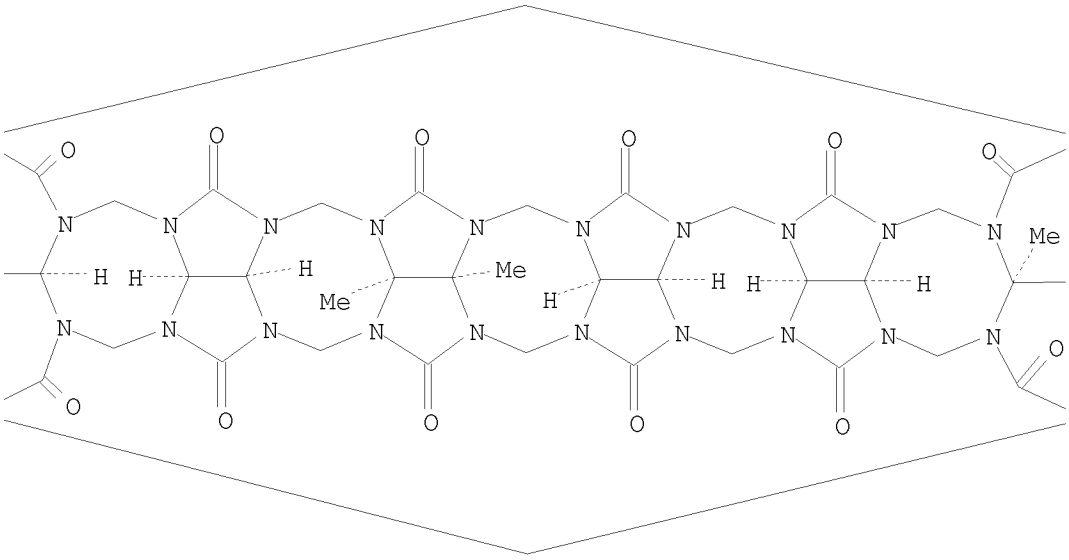


IT 848440-56-2, α,α',δ,δ'-
Tetramethylcucurbit[6]uril
RL: RCT (Reactant); RACT (Reactant or reagent)
(proton transfer reaction with glutamic acid)
RN 848440-56-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

PAGE 1-B



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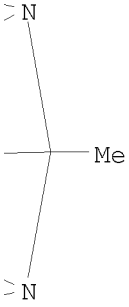


REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:871648 CAPLUS
DOCUMENT NUMBER: 151:268504
TITLE: Remarkable salt effect on stability of supramolecular complex between modified cucurbit[6]uril and methylviologen in aqueous media
AUTHOR(S): Khan, Muhammad S. A.; Heger, Dominik; Necas, Marek; Sindelar, Vladimir

CORPORATE SOURCE: Department of Chemistry, Masaryk University, Brno, 611 37, Czech Rep.
SOURCE: Journal of Physical Chemistry B (2009), 113(32), 11054-11057
CODEN: JPCBFK; ISSN: 1520-6106
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 151:268504

AB The supramol. complex formed by partial inclusion of methylviologen in hexamethylated cucurbit[6]uril was described both in solution and in the solid state. The association constant of the complex was determined using 1H NMR and UV-visible spectrophotometric titration An extraordinary 2000-fold drop in the association constant of the complex was observed when pure water was replaced by 50 mM NaCl solution

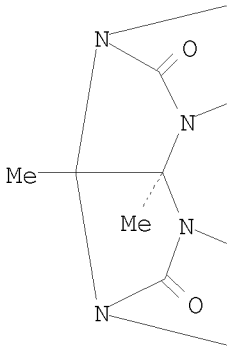
IT 1179529-29-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; salt effect on stability of supramol. complex between methylated cucurbit[6]uril and methylviologen in aqueous media)
RN 1179529-29-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

CM 1

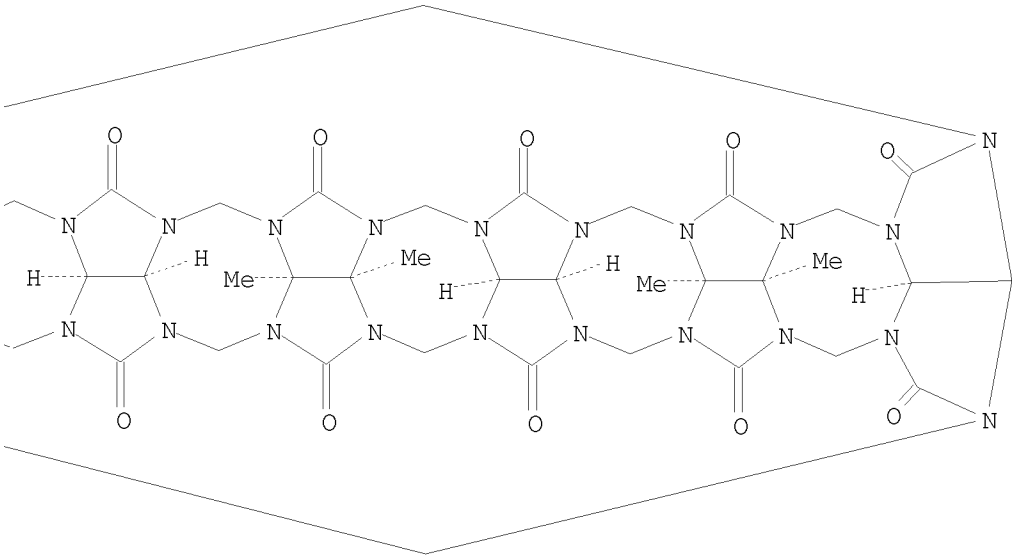
CRN 640732-36-1
CMF C42 H48 N24 O12

Relative stereochemistry.

PAGE 1-A

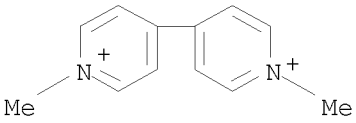


PAGE 1-B



CM 2

CRN 1910-42-5
CMF C12 H14 N2 . 2 Cl



●2 Cl^-

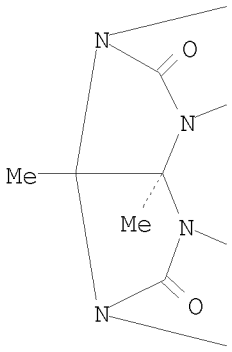
IT 1179529-30-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; salt effect on stability of supramol. complexes of methylated cucurbit[6]uril in aqueous media)
RN 1179529-30-6 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

CM 1

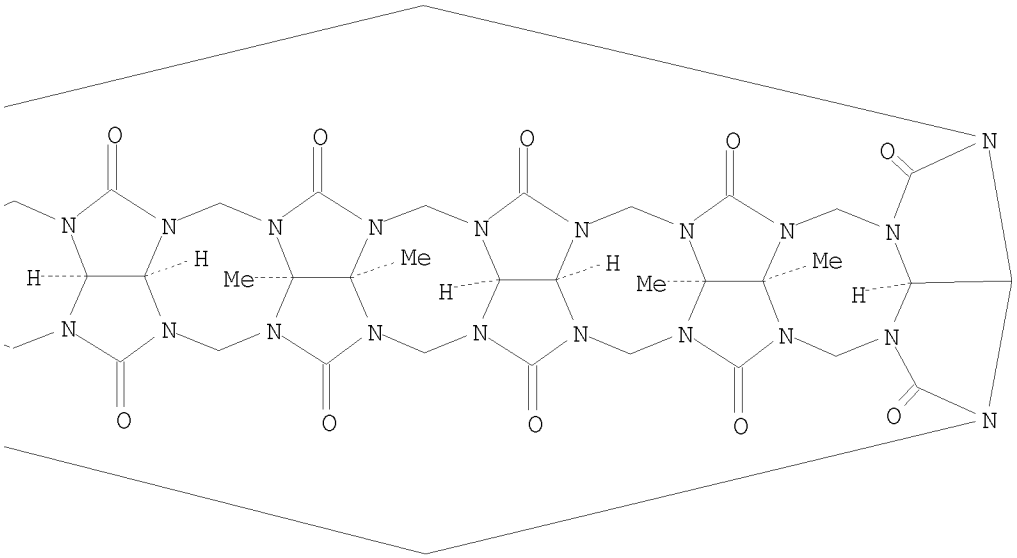
CRN 640732-36-1
CMF C42 H48 N24 O12

Relative stereochemistry.

PAGE 1-A

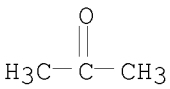


PAGE 1-B



CM 2

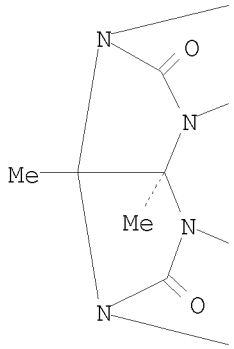
CRN 67-64-1
CMF C3 H6 O



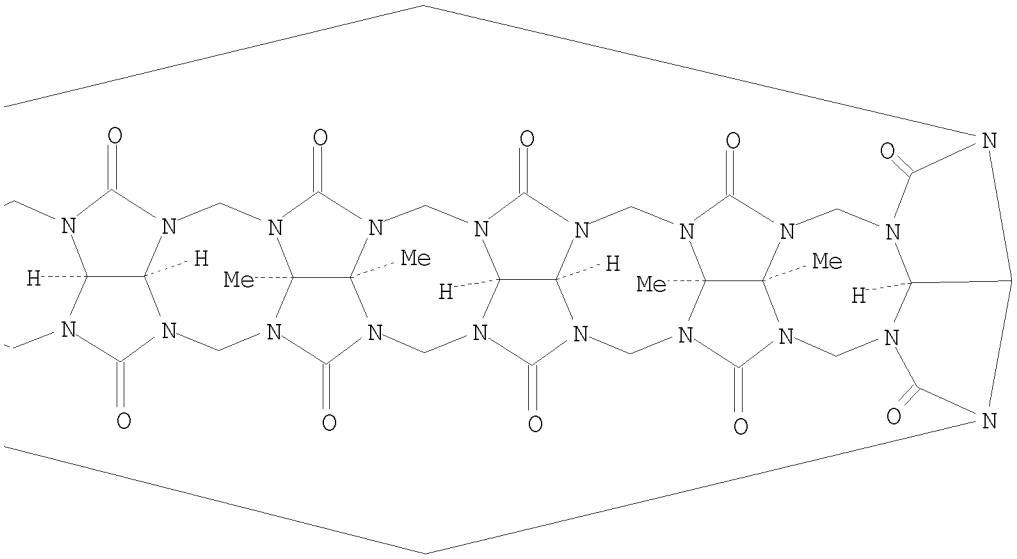
IT 640732-36-1
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(salt effect on stability of supramol. complex between methylated cucurbit[6]uril and methylviologen in aqueous media)
RN 640732-36-1 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,19b,19c,23b,23c,26b-hexamethyl-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:784522 CAPLUS
DOCUMENT NUMBER: 151:172810
TITLE: Crystal structures of three host-guest complexes of methyl-substituted cucurbit[6]urils and anthracene derivatives
AUTHOR(S): Chen, Ze-Hua; Zhou, Fa-Geng; Zhang, Yun-Qian; Zhu, Qian-Jiang; Xue, Sai-Feng; Tao, Zhu
CORPORATE SOURCE: Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Journal of Molecular Structure (2009), 930(1-3), 140-146
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 151:172810
AB Three host-guest complexes of methyl-substituted cucurbit[6]uril hosts and anthracene derivs. guests were synthesized and structurally characterized by single crystal x-ray diffractions and 1H NMR technique. The hosts are dodecamethylcucurbit[6]uril (DDMeQ[6]), α,α',δ,δ'-tetramethylcucurbit[6]uril (TMeQ[6]), and hexa-methylsubstituted cucurbituril (HSMeQ[6]) made from 3a-methylglycoluril. The guests are 9,10-bis[N-(2-aminoethyl)aminomethyl]anthracene (AN1), 9,10-bis[N-(3-aminopropyl)aminomethyl]anthracene (AN2) and 9,10-bis[N-(4-aminobutyl)aminomethyl]anthracene (AN3). The crystal structures show the compds. 1-3 with stoichiometry of {DDMeQ[6]-AN1}2+2NO3-.24H2O (1), {TMeQ[6]-AN2}2+4NO3- 2H3O+.10H2O (2) and

{2HSMeQ[6]-AN3}2+2Cl-.25H2O (3) resp., and the formation of an exclusion or inclusion host-guest complex is dependent on the length of the substituted alkyl chains on the anthracene.

IT 848440-56-2
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(complexation with aminoalkylated anthracenes; crystal structures of three host-guest complexes of methyl-substituted cucurbit[6]urils and aminoalkylated anthracenes)

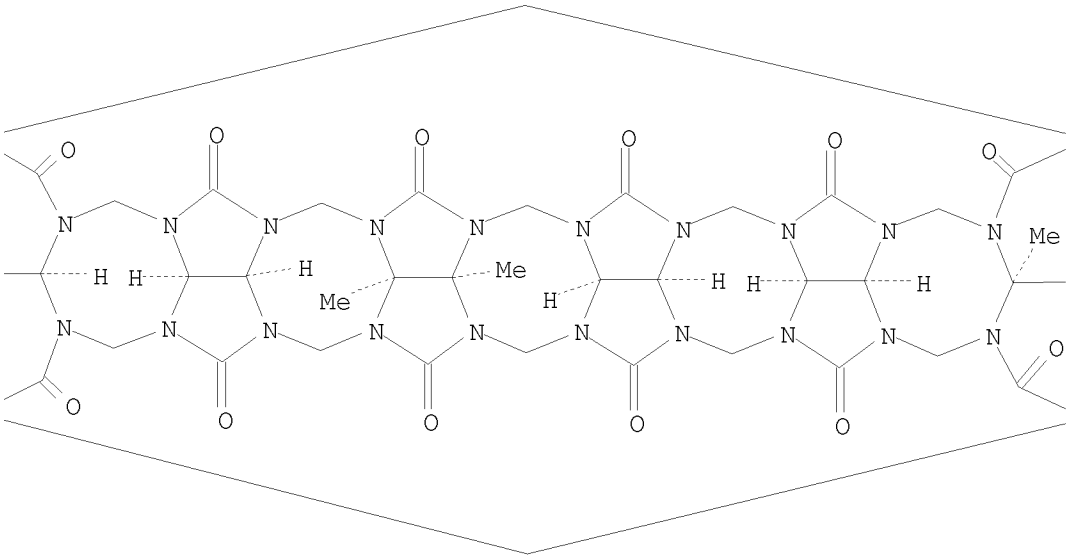
RN 848440-56-2 CAPLUS

CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

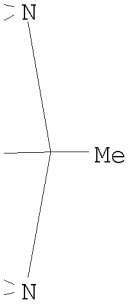
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



IT 1173288-20-4P
RL: NANO (Nanomaterial); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(nanocapsule, crystallog.; crystal structures of three host-guest complexes of methyl-substituted cucurbit[6]urils and aminoalkylated anthracenes)

RN 1173288-20-4 CAPLUS

CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2''

,3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer, compd. with N9,N10-bis(3-aminopropyl)-9,10-anthracenedimethanamine, nitrate, hydrate (1:1:4:12) (CA INDEX NAME)

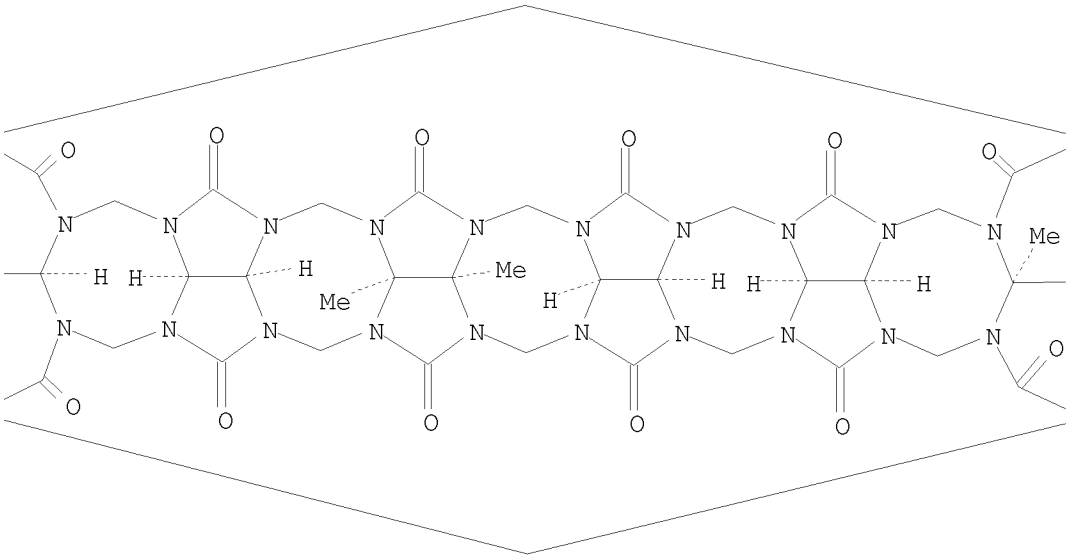
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

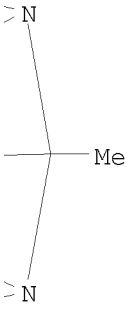
Relative stereochemistry.

PAGE 1-A

PAGE 1-B

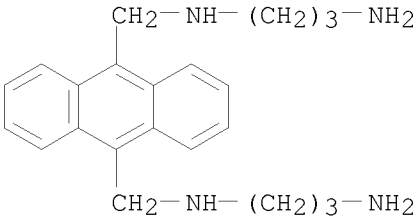


PAGE 1-C



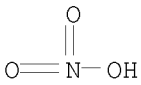
CM 2

CRN 127997-41-5
CMF C22 H30 N4



CM 3

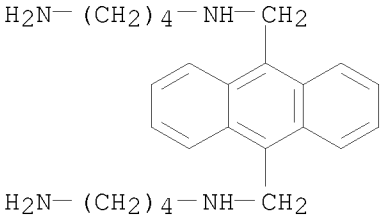
CRN 7697-37-2
CMF H N O3



IT 1173288-23-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(pseudorotaxane; crystal structures of three host-guest complexes of methyl-substituted cucurbit[6]urils and aminoalkylated anthracenes)
RN 1173288-23-7 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer, compd. with
N9,N10-bis(4-aminobutyl)-9,10-anthracenedimethanamine, hydrochloride
(1:1:2) (CA INDEX NAME)

CM 1

CRN 1116511-60-4
CMF C24 H34 N4



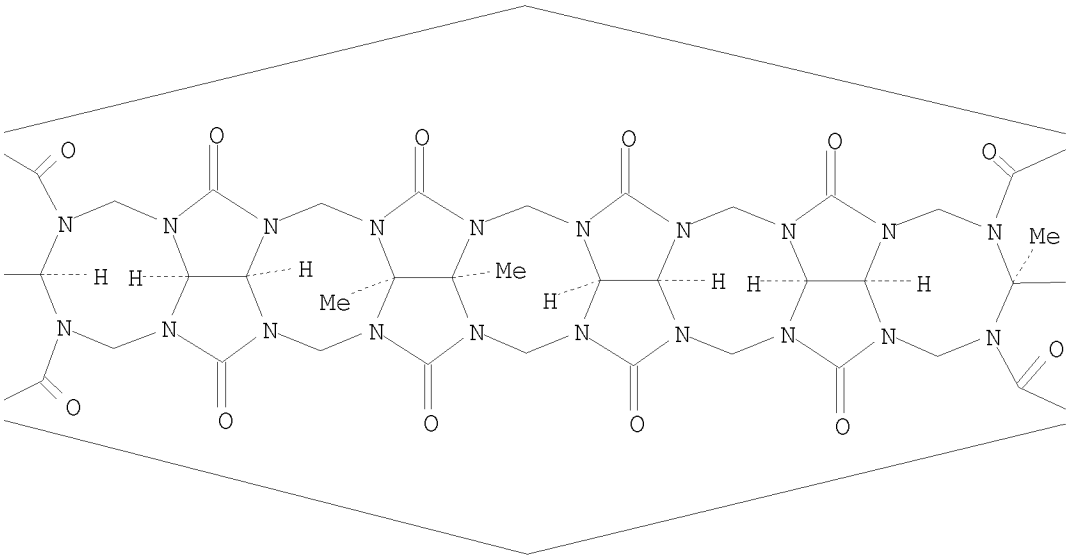
CM 2

CRN 848440-56-2
CMF C40 H44 N24 O12

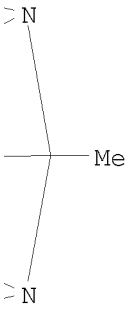
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



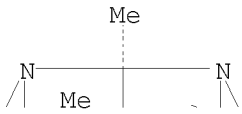
REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:690210 CAPLUS
DOCUMENT NUMBER: 151:259055
TITLE: Molecular capsules formed by three different cucurbit[5]urils and some lanthanide ions
AUTHOR(S): Zhang, Yun-Qian; Zeng, Jin-Ping; Zhu, Qian-Jiang; Xue, Sai-Feng; Tao, Zhu
CORPORATE SOURCE: Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Journal of Molecular Structure (2009), 929(1-3), 167-173
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 151:259055
AB Four mol. capsules based on three different cucurbit[5]urils, which are Di-Me cucurbit[5]uril (DMeQ[5]), decamethylcucurbit[5]uril (Me10Q[5]) and the normal cucurbit[5]uril, were synthesized and structurally characterized by single-crystal x-ray diffractions. They are {[Gd2(H2O)9][DMeQ[5]@Cl]}5+.cntdot.5Cl-.cntdot.13(H2O) (1), {[Nd2(H2O)8Cl][Me10Q[5]@Cl]}4+.cntdot.4Cl-.cntdot.9(H2O) (2), {K(H2O)2Cl·{[Dy2(H2O)6Cl][Q[5]@Cl]}2}8+.cntdot.2{[Dy2(H2O)7Cl][Q[5]@Cl]}4+.cntdot.16Cl-.cntdot.44(H2O) (3) and 2{[Y2(H2O)8][Me10Q[5]@Cl]}5+.cntdot.10Cl-.cntdot.48(H2O) (4). In the crystal structure of these compds., mol. capsules included a Cl- anion and lidded with lanthanide cations were observed
IT 569359-77-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of rare earth cucurbit[5]uril aqua chloro dinuclear capsule complexes)
RN 569359-77-9 CAPLUS
CN 1H,4H,12H,15H-2,14:3,13-Dimethano-

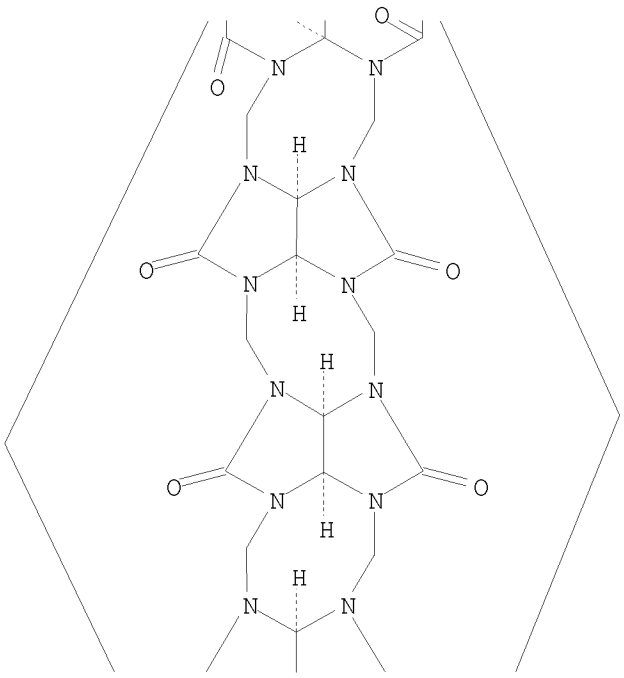
5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pe
ntaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,22b-dimethyl-, stereoisomer
(CA INDEX NAME)

Relative stereochemistry.

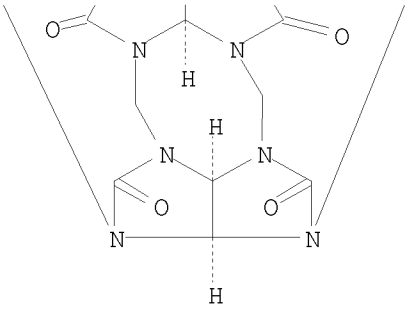
PAGE 1-A



PAGE 2-A



PAGE 3-A



REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:604078 CAPLUS
DOCUMENT NUMBER: 151:162497
TITLE: Molecular capsules based on methyl-substituted cucurbit[5]urils and strontium-capped
AUTHOR(S): Zhou, Fa-Gen; Wu, Li-Hui; Lu, Xiao-Jun; Zhang, Yun-Qian; Zhu, Qian-Jiang; Xue, Sai-Feng; Tao, Zhu
CORPORATE SOURCE: Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang, 550025, Peop. Rep. China

SOURCE: Journal of Molecular Structure (2009), 927(1-3), 14-20
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 151:162497

AB Four mol. capsules based on three Me-substituted cucurbit[5]urils, which are α,β,δ-hexamethylcucurbit[5]uril (α,β,δ-HMeQ[5]), decamethylcucurbit[5]uril (Me10Q[5]) and a pentamethylcucurbit[5]uril constructed of a monomethyl-glycouril (PMeQ[5]), were synthesized and structurally characterized by single crystal x-ray diffractions. They are {[α,β,.delta.-HMeQ[5]@Cl][Sr(H2O)2]2}3+Cl-3·13(H2O) (1), {[α,β,.delta.-HMeQ[5]@(NO3)][Sr(NO3)(H2O)]2}+[NO3]-HNO3·4(H2O) (2), {[Me10Q[5]@(NO3)][Sr(NO3)(H2O)]2}+(NO3)-·8(H2O) (3) and {[PMeQ[5]@Cl][Sr(H2O)2]2}3+Cl-3·22(H2O) (4). In the crystal structure of these compds., mol. capsules included a Cl- or a NO3- anion and lidded with strontium cations were observed

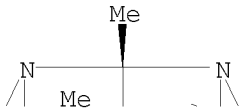
IT 1045894-48-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of strontium dinuclear mol. capsule complexes with methyl-substituted cucurbit[5]urils)

RN 1045894-48-1 CAPLUS

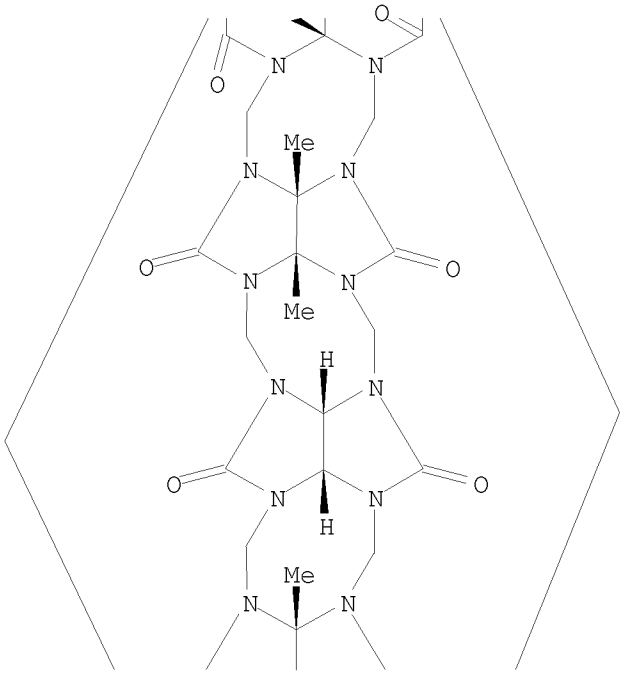
CN 1H,4H,12H,15H-2,14:3,13-Dimethano-5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,17b,17c,21b,21c,22b-hexamethyl-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

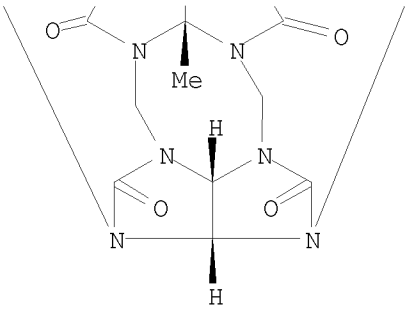
PAGE 1-A



PAGE 2-A



PAGE 3-A



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:452729 CAPLUS
DOCUMENT NUMBER: 152:74578
TITLE: Host-guest complexes of a water soluble cucurbit[6]uril derivative with some dications of 1,ω-alkyldipyridines: 1H NMR and X-ray structures
AUTHOR(S): Xiao, Xin; Zhang, Yun Qian; Zhu, Qian Jiang; Xue, Sai Feng; Tao, Zhu
CORPORATE SOURCE: Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Science in China, Series B: Chemistry (2009), 52(4), 475-482
CODEN: SCBCFQ; ISSN: 1006-9291
PUBLISHER: Science in China Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Interactions between a sym. tetramethyl-substituted cucurbit[6]uril (host: TMeQ[6]) and 1,ω-alkylenedipyridine (ω = 2, 4, 6, 8, 10) dicationic guests were studied using 1H NMR spectroscopy and single crystal x-ray crystallog. In these inclusion complexes, combined cavity and portal binding in TMeQ[6] were observed, and the length of the bridged alkylene was found to play an important role not only in balancing the overall hydrophilic/hydrophobic interaction between the host and the guest, but also in defining the structure of the resulting inclusion complexes. For the guest 1,2-ethylenedipyridine (Edpy), TMeQ[6] includes a pos. charged pyridine ring of Edpy to form an unsym. inclusion complex; for the guest 1,4-butylenedipyridine (Bdpy), TMeQ[6] includes a pos. charged pyridine ring of Bdpy, but the different competitive interactions in and between the related inclusion complexes could lead to a fast exchange between the hosts and guests. For the guests with longer bridge chains, such as 1,6-hexamethylenedipyridine (Hdpy) or 1,8-octylenedipyridine (Odpy), a stable pseudorotaxane inclusion complex is formed by combining the hydrophobic cavity and the outer portal dipole-ion interactions. However, for 1,10-decatylenedipyridine (Ddpy), the two TMeQ[6] host mols. include the two end pyridine rings of Ddpy and form a dumbbell inclusion complex.

IT 1201815-11-3 1201815-12-4
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(1H NMR and X-ray structures of host-guest complexes of water soluble cucurbit[6]uril derivative with e dications N,N'- 1,ω-alkyldipyridium bromides)
RN 1201815-11-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

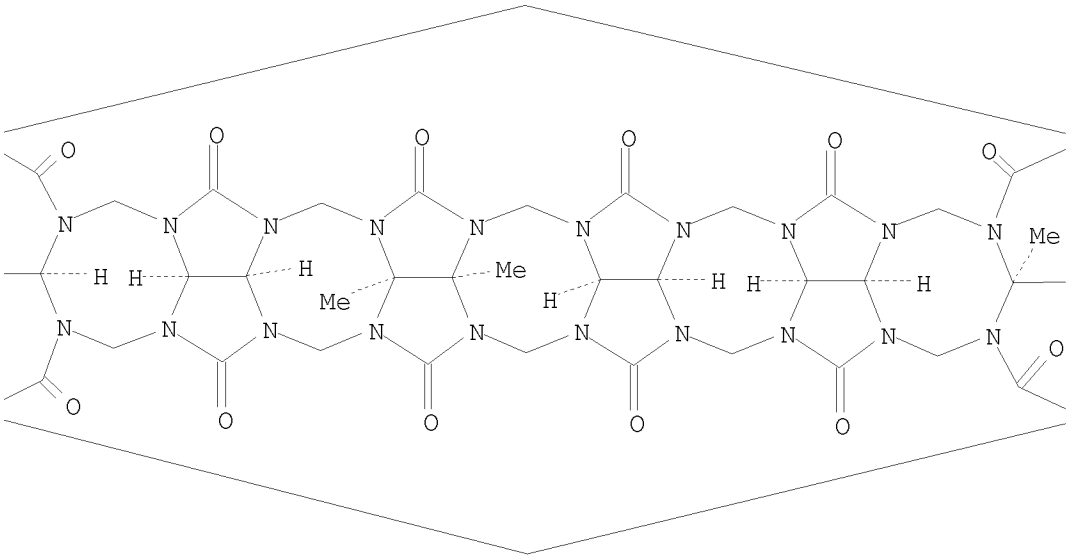
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

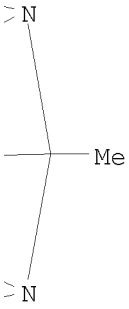
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



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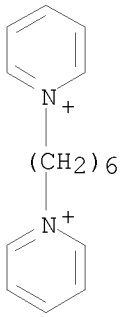
CRN 53952-75-3
CMF C16 H22 N2 . 2 Br



●2 Br^-

RN 1201815-12-4 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

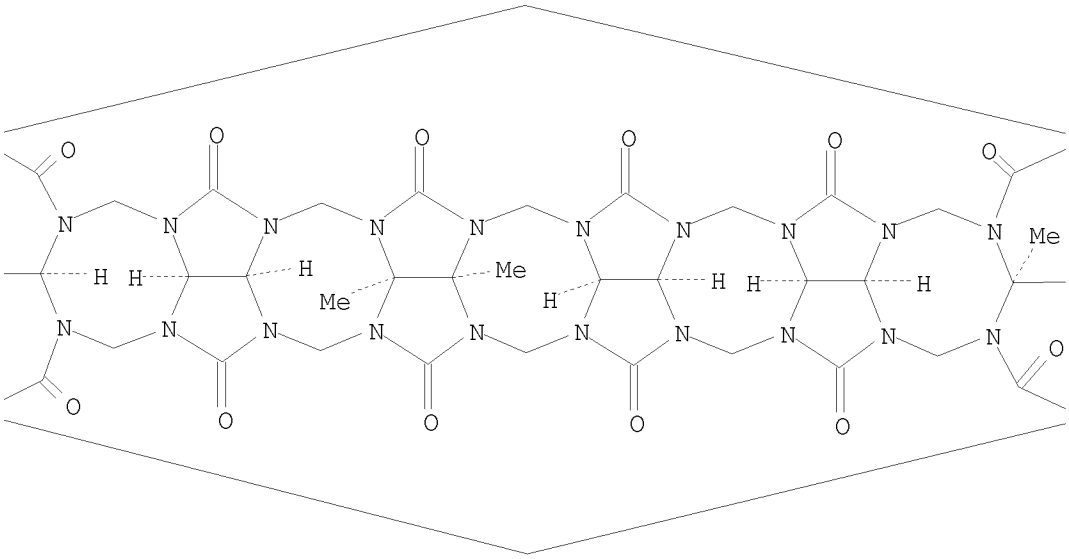
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

Relative stereochemistry.

PAGE 1-A

PAGE 1-B



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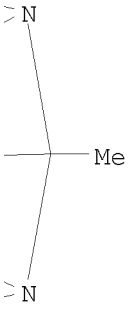
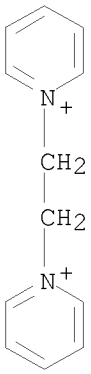


CM 2

CRN 882-35-9
CMF C12 H14 N2 . 2 Br



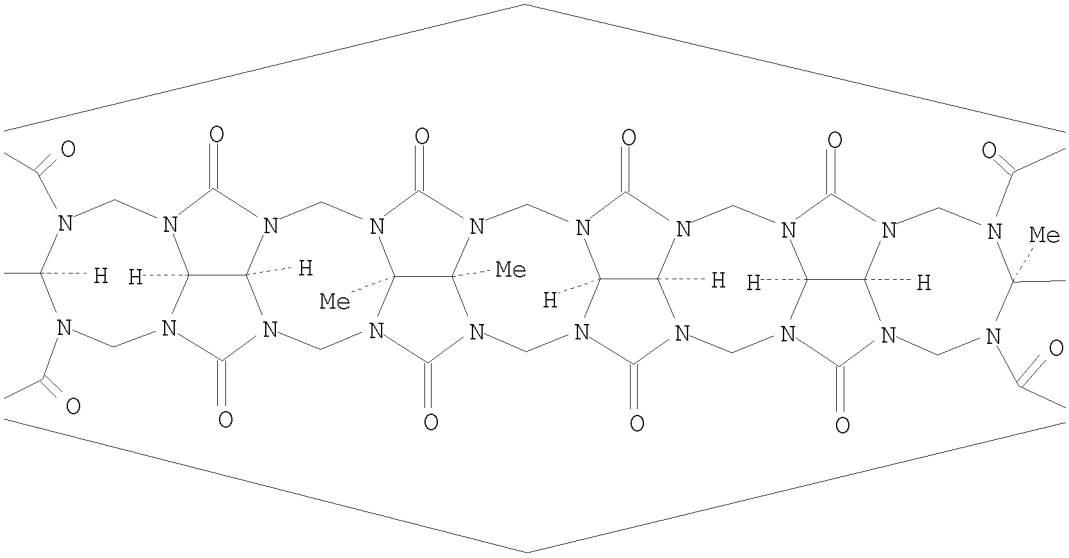
●2 Br^-

IT 848440-56-2
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(1H NMR and X-ray structures of host-guest complexes of water soluble cucurbit[6]uril derivative with e dications N,N'- 1,ω-alkyldipyridium bromides)
RN 848440-56-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

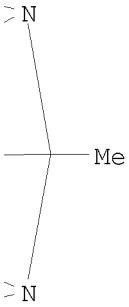
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



IT 1201815-08-8P 1201815-09-9P 1201815-10-2P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(1H NMR and X-ray structures of host-guest complexes of water soluble cucurbit[6]uril derivative with e dications N,N'- 1,ω-alkyldipyridium bromides)
RN 1201815-08-8 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

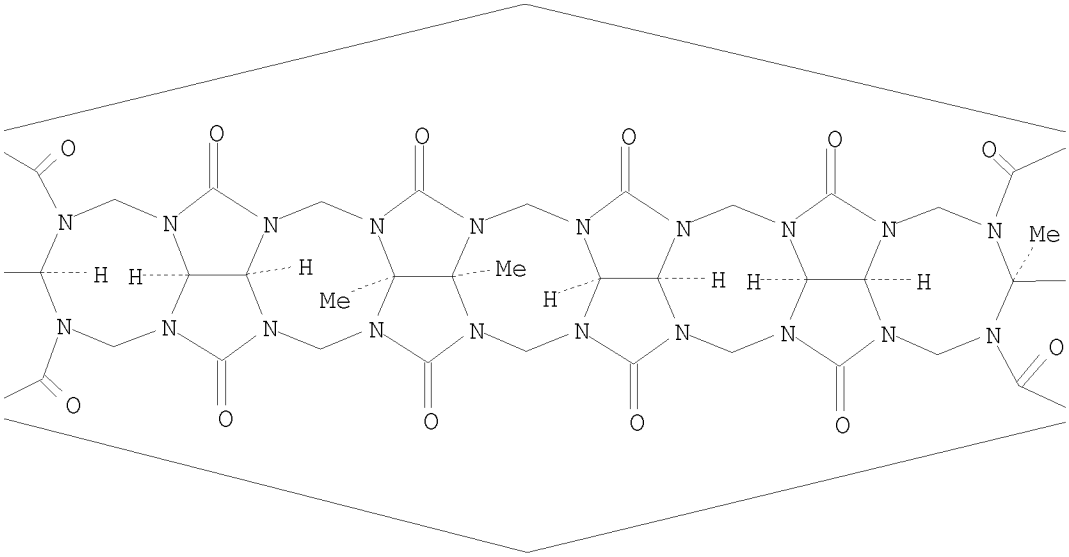
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

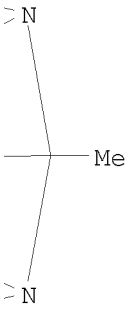
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



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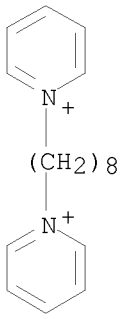
CRN 32405-53-1
CMF C18 H26 N2 . 2 Br



●2 Br^-

RN 1201815-09-9 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

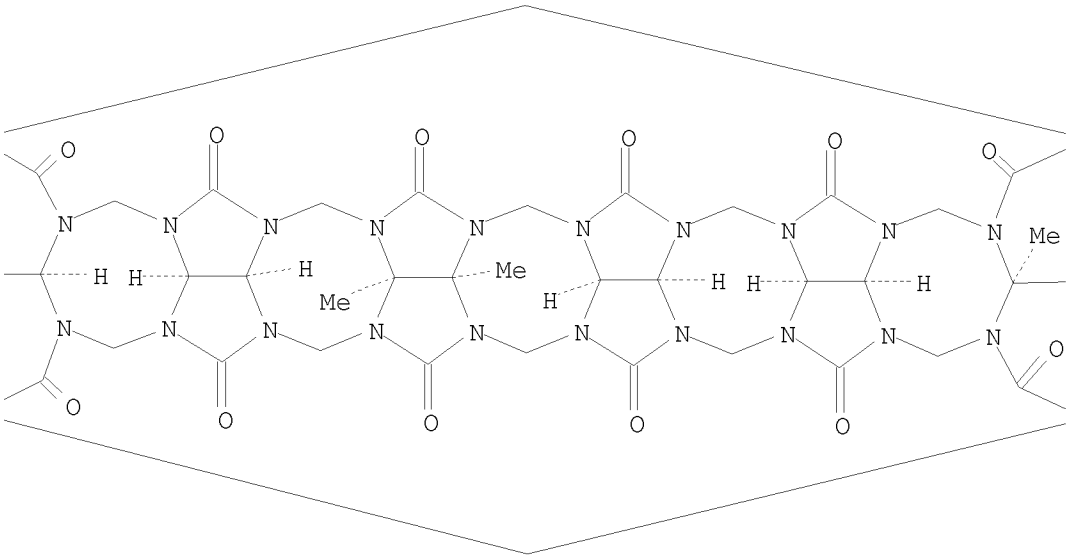
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

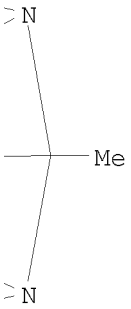
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



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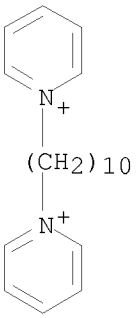
CRN 6266-40-6
CMF C20 H30 N2 . 2 Br



●2 Br^-

RN 1201815-10-2 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

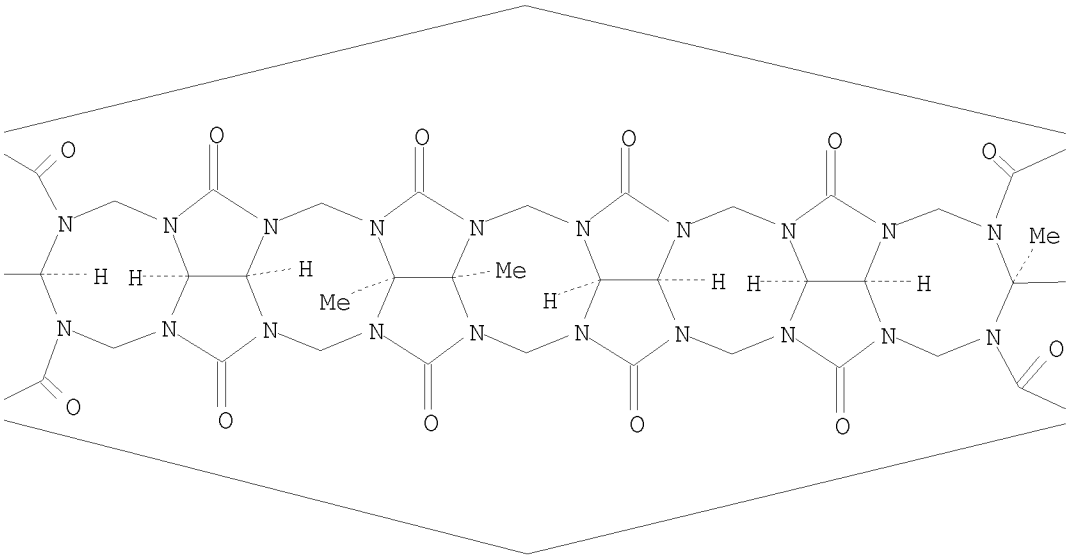
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

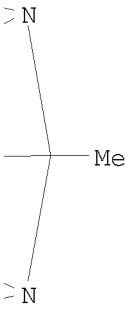
Relative stereochemistry.

PAGE 1-A

PAGE 1-B

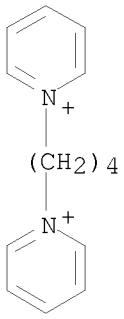


PAGE 1-C



CM 2

CRN 14208-08-3
CMF C14 H18 N2 . 2 Br



●2 Br^-

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:1428646 CAPLUS
DOCUMENT NUMBER: 150:472123
TITLE: Structure of supramolecular assemblies formed by α,δ-tetramethylcucurbit[6]uril and 4-nitrophenol
AUTHOR(S): Zheng, Li-Mei; Zhang, Yun-Qian; Zeng, Jin-Ping; Qiu, Yan; Yu, Da-Hai; Xue, Sai-Feng; Zhu, Qian-Jiang; Tao, Zhu

CORPORATE SOURCE: School of Chemistry and Chemical Engineering, Henan University of Technology, Zhengzhou, 450001, Peop. Rep. China
SOURCE: Molecules (2008), 13(11), 2814-2822
CODEN: MOLEFW; ISSN: 1420-3049
URL: http://www.mdpi.com/1420-3049/13/11/2814/pdf
PUBLISHER: Molecular Diversity Preservation International
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English

AB A host-guest assembly, [(C40H44N24O12)·(C6H5 NO3)8·13(H2O)] (1), based on a partial substituted cucurbituril, α,δ-tetramethylcucurbit[6]uril (TMeQ[6]), and 4-nitrophenol was synthesized and structurally characterized by single-crystal X-ray diffraction. A combination of hydrogen-bonding between the latticed water mol. and the hydroxyl group of 4-nitrophenol, the hydroxyl group of 4-nitrophenol and the carbonyl groups lining the portals in addition, the C-H···π interactions between the 4-nitrophenol mols. could be the driving forces of formation such an exclusion host-guest assembly.

IT 1146689-24-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; structure of supramol. assemblies formed by α,δ-tetramethylcucurbit[6]uril and 4-nitrophenol)

RN 1146689-24-8 CAPLUS

CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer, compd. with nitrobenzene, hydrate (1:8:13) (CA INDEX NAME)

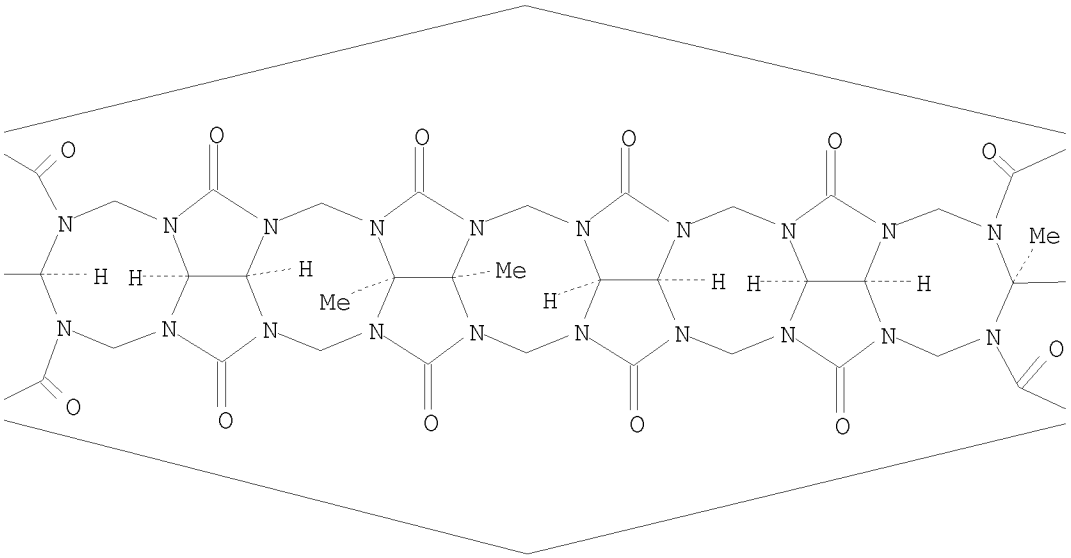
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

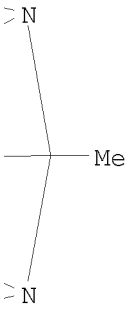
Relative stereochemistry.

PAGE 1-A

PAGE 1-B

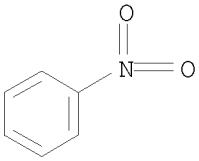


PAGE 1-C



CM 2

CRN 98-95-3
CMF C6 H5 N O2

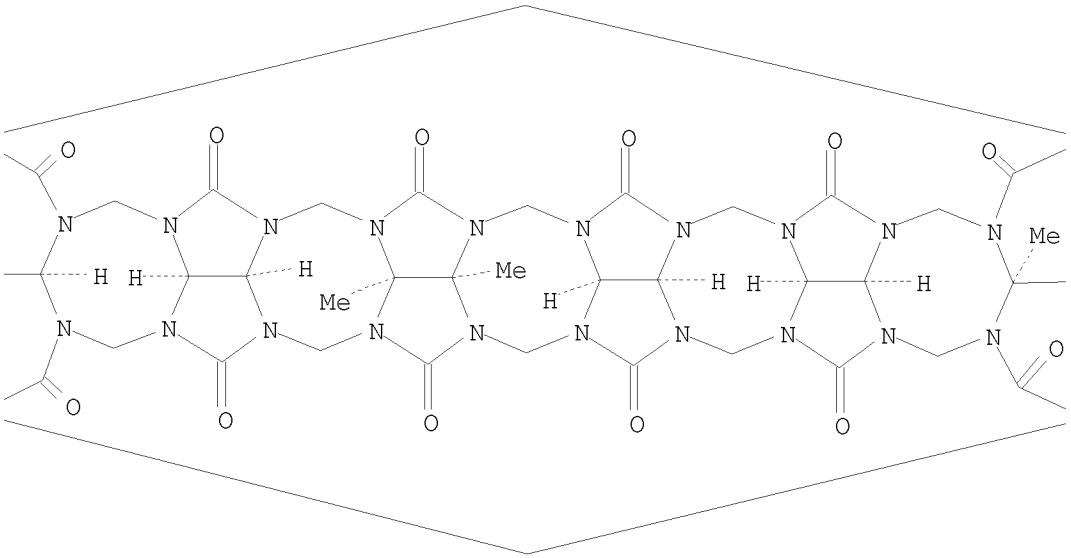


IT 848440-56-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(structure of supramol. assemblies formed by
α,δ-tetramethylcucurbit[6]uril and 4-nitrophenol)
RN 848440-56-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

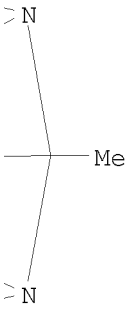
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:1372317 CAPLUS
DOCUMENT NUMBER: 150:55645
TITLE: Host-guest inclusion complexes of four partial alkyl-substituted cucurbit[6]urils with some probe guests
AUTHOR(S): Yu, Da-Hai; Ni, Xin-Long; Tian, Zhong-Cheng; Zhang, Yun-Qin; Xue, Sai-Feng; Tao, Zhu; Zhu, Qing-Jiang
CORPORATE SOURCE: Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Journal of Molecular Structure (2008), 891(1-3), 247-253
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 150:55645
AB Using probe guests, three host-guest inclusion complexes of two new alkyl-substituted cucurbit[6]uril hosts, ortho-tetramethyl cucurbit[6]uril (o-TMeQ[6]) and sym. tetracyclohexano cucurbit[6]uril (TCyHQ[6]) have been characterized successfully by single crystal X-ray diffractions. They are {o-TMeQ[6]-5,5'dimethyl-2,2'-bispyridine (DMBPY.H)+}Cl-21H2O(1), {(o-TMeQ[6])2-1,6-bisbenzoimidazolylhexane (SBH.2H)2+} 2Cl-52H2O (2) and {TCyHQ[6]-dioxane}14H2O (3). Moreover, two similar crystal structure of two inclusion complexes of other two partial substituted cucurbit[6]urils, meta-hexamethyl cucurbit[6]uril (m-HMeQ[6]) and sym. dicyclohexano cucurbit[6]uril (p-(CyH)2Q[6]) with HCl salt of DMBPY were also reported. They were {p-(CyH)2Q[6]-DMBPY +}Cl-16H2O (4) and {m-HMeQ[6]-DMBPY +}Cl-15H2O (5). The driving force for the information of the host-guest inclusion complexes can be attributed to not only the cavity interaction (host), but also the hydrogen bonding and ion-dipole interaction between

the carbonyl oxygen at the portals of the host and the protonated nitrogen of the guest.

IT 1092792-08-9P 1092792-09-0P 1092792-10-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystallog.; host-guest inclusion complexes of four partial alkyl-substituted cucurbit[6]urils with some probe guests)

RN 1092792-08-9 CAPLUS

CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,25b,25c,26b-tetramethyl-, stereoisomer, compd. with 5,5'-dimethyl-2,2'-bipyridine, hydrochloride, hydrate (1:1:1:21) (CA INDEX NAME)

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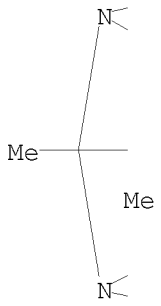
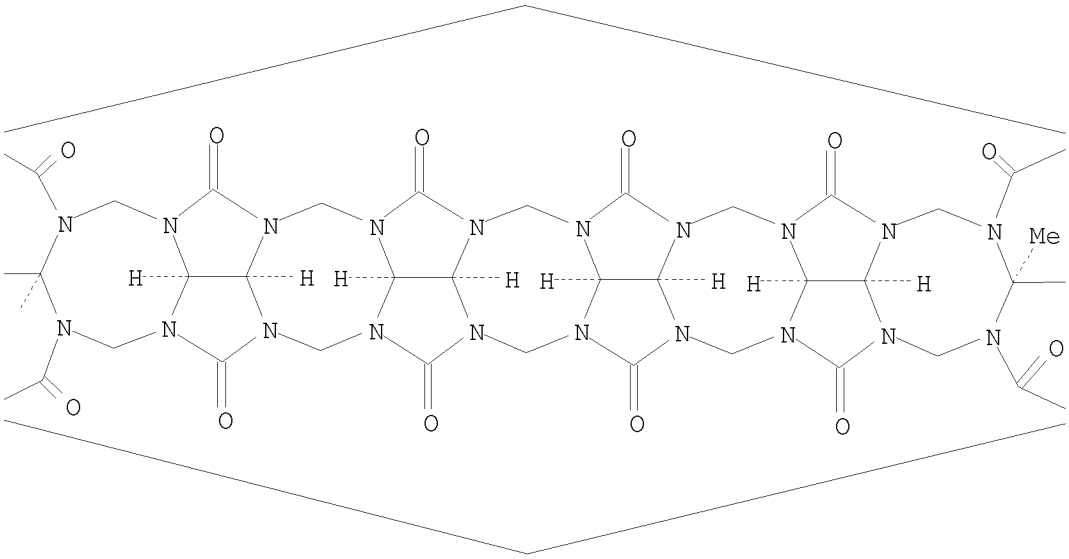
CRN 1092792-07-8
CMF C40 H44 N24 O12

Relative stereochemistry.

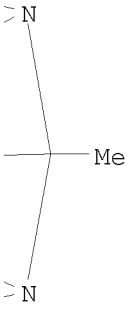
PAGE 1-A



PAGE 1-B



PAGE 1-C



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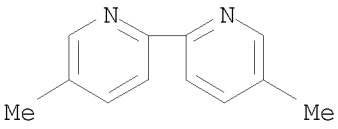

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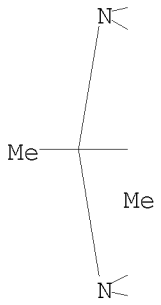
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,25b,25c,26b-tetramethyl-, stereoisomer, compd. with
2,2'-(1,6-hexanediyl)bis[1H-benzimidazole], hydrochloride, hydrate
(2:1:2:52) (CA INDEX NAME)

CM 1

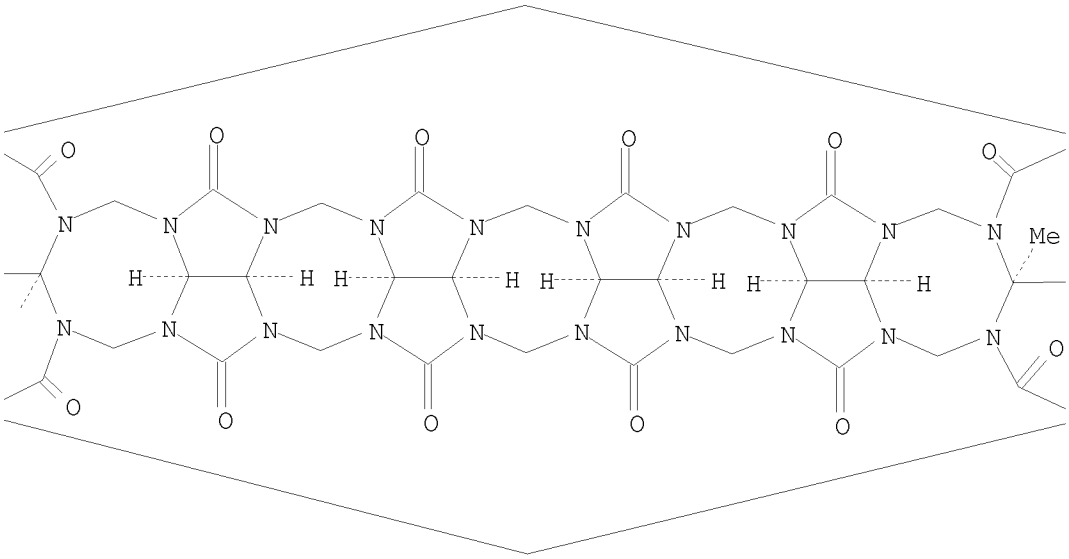
CRN 1092792-07-8
CMF C40 H44 N24 O12

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



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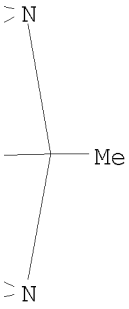

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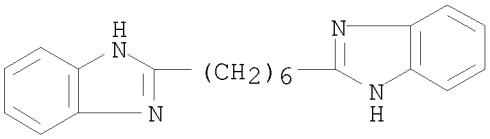

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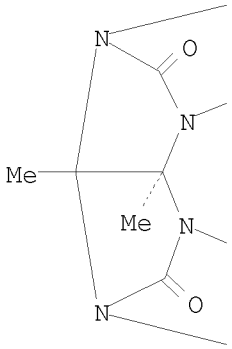
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24
a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2''
,3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-
g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,19b,19c,23b,23c,26b-hexamethyl-, stereoisomer, compd. with
5,5'-dimethyl-2,2'-bipyridine, hydrochloride, hydrate (1:1:1:15) (CA
INDEX NAME)

CM 1

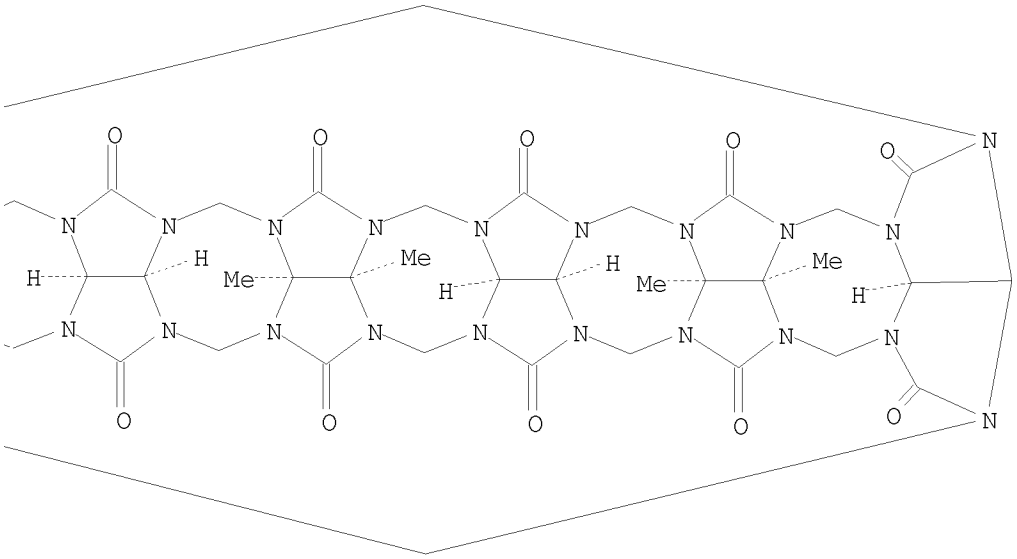
CRN 640732-36-1
CMF C42 H48 N24 O12

Relative stereochemistry.

PAGE 1-A

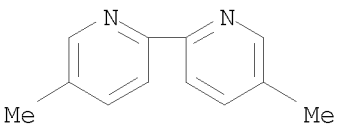


PAGE 1-B



CM 2

CRN 1762-34-1
CMF C12 H12 N2

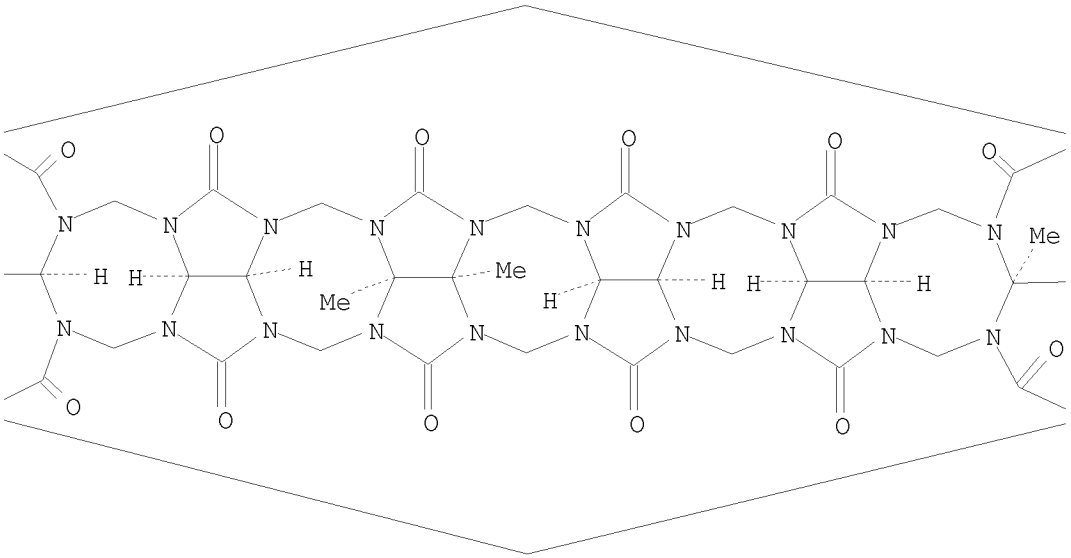


IT 848440-56-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(host, inclusion reaction; host-guest inclusion complexes of four partial alkyl-substituted cucurbit[6]urils with some probe guests)
RN 848440-56-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

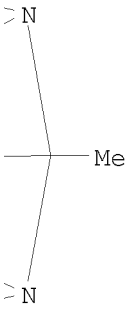
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:1198526 CAPLUS
DOCUMENT NUMBER: 149:493259
TITLE: Interaction models of three alkyl substituted cucurbit[6]urils with a hydrochloride salt of 4,4'-dipyridyl guest
AUTHOR(S): Tian, Zhong-Cheng; Ni, Xin-Long; Xiao, Xin; Wu, Feng; Zhang, Yun-Qian; Zhu, Qian-Jiang; Xue, Sai-Feng; Tao, Zhu
CORPORATE SOURCE: Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Journal of Molecular Structure (2008), 888(1-3), 48-54
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Three host-guest complexes, {(H2O)2@(CyH)2Q[6]} (4,4'-bpyH)+·Cl-·10H2O (1), {(1,4-dioxane)@m-TriCyHQ[6]}(4,4'-bpyH)+·Cl-·19H2O (2), {(4,4'-bpyH2)2+@TMeQ[6]}.cntdot.2Br-.cntdot.11H2O (3), were prepared with three different alkyl substituted cucurbit[6]urils, sym. dicyclohexanocucurbit[6]uril {(CyH)2Q[6]}, meta tricyclohexanocucurbit[6]uril (m-TriCyHQ[6]), sym. tetramethylcucurbit[6]uril (TMeQ[6]), and a HCl salt 4,4'-dipyridyl(4,4'-bpyHCl) or a HBr salt 4,4'-dipyridyl[4,4-bpy(HBr)2] guest. Their crystal structures characterized by single-crystal X-ray diffractions revealed that these hosts can form supramol. assemblies with the halogen hydride salts of the guest 4,4'-bpy through the ion-dipole interaction, hydrogen bonding, C-H···π or N-H···π interaction and π···π stacking. The substituted alkyl group

could affect the interaction model and assembled characteristic of the host and the guest.

IT 1072627-22-5P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(crystallog.; interaction models of three alkyl substituted cucurbit[6]urils with hydrochloride salt of 4,4'-dipyridyl guest)

RN 1072627-22-5 CAPLUS

CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer, compd. with 4,4'-bipyridine, hydrobromide, hydrate (1:1:2:11) (CA INDEX NAME)

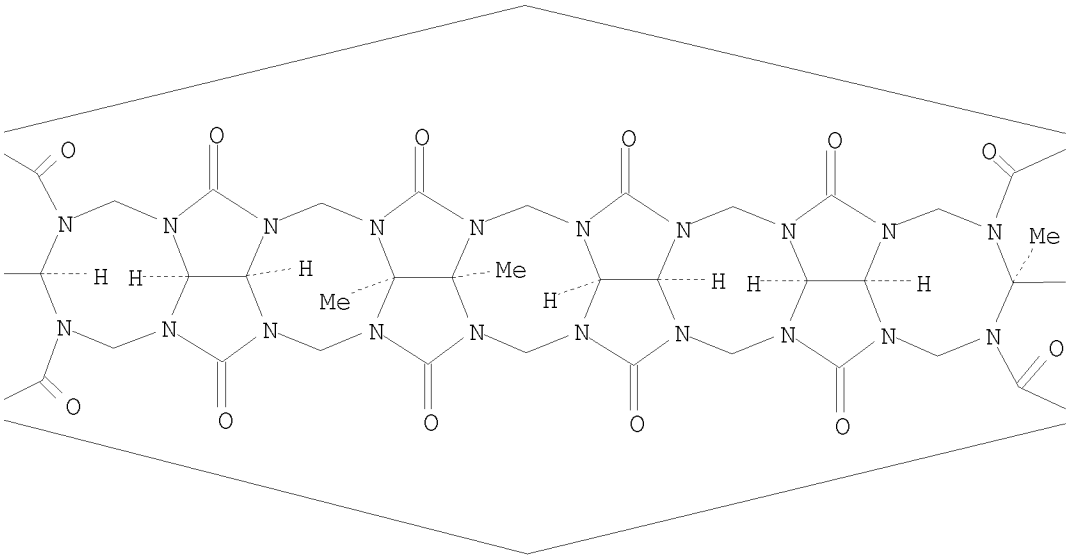
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

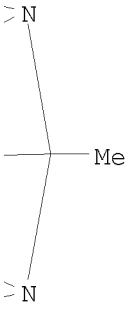
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



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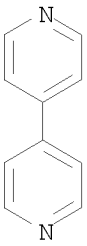
CRN 553-26-4
CMF C10 H8 N2



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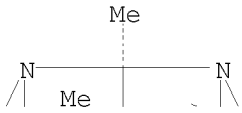
REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:928382 CAPLUS
DOCUMENT NUMBER: 149:322413
TITLE: Supramolecular Bracelets and Interlocking Rings Elaborated Through the Interrelationship of Neighboring Chemical Environments of Alkyl-Substitution on Cucurbit[5]uril
AUTHOR(S): Ni, Xin-Long; Lin, Jing-Xiang; Zheng, Yu-Ying; Wu, Wen-Shi; Zhang, Yun-Qian; Xue, Sai-Feng; Zhu, Qian-Jiang; Tao, Zhu; Day, Anthony I.
CORPORATE SOURCE: Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang, Guizhou, 550025, Peop. Rep. China
SOURCE: Crystal Growth & Design (2008), 8(9), 3446-3450 CODEN: CGDEFU; ISSN: 1528-7483
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:322413
AB The smallest members of the cucurbituril family, cucurbit[5]uril (L1) and the alkyl-cucurbit[5]urils α,α'-dimethylcucurbit[5]uril (L2) and α,β,δ-tricyclohexanylcucurbit[5]uril (L3), can be used as a building blocks, linked by metal ions to create supramol. rings. Three supramol. complexes, {K2(H2O@L1)}[InCl4(H2O)2]·4.5H2O, {Sr2(Cl@L2)}Cl3·19H2O and {K3(H2O@L3)}Cl2·15.5H2O, were characterized by x-ray crystallog. The cavities found at the center of these rings have dimensions between 7 and 19 Å in width and 8.5 Å in depth. The partially substituted alkyl-cucurbit[5]urils present the most interesting supramol. ring formation. This occurs as a result of selective coordination of metal ions to the carbonyl oxygens of the glycoluril moieties carrying alkyl substitution.
IT 569359-77-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of potassium aqua and strontium chloro supramol. complexes with cucurbit[5]uril and alkyl-cucurbit[5]urils)
RN 569359-77-9 CAPLUS
CN 1H,4H,12H,15H-2,14:3,13-Dimethano-5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pe

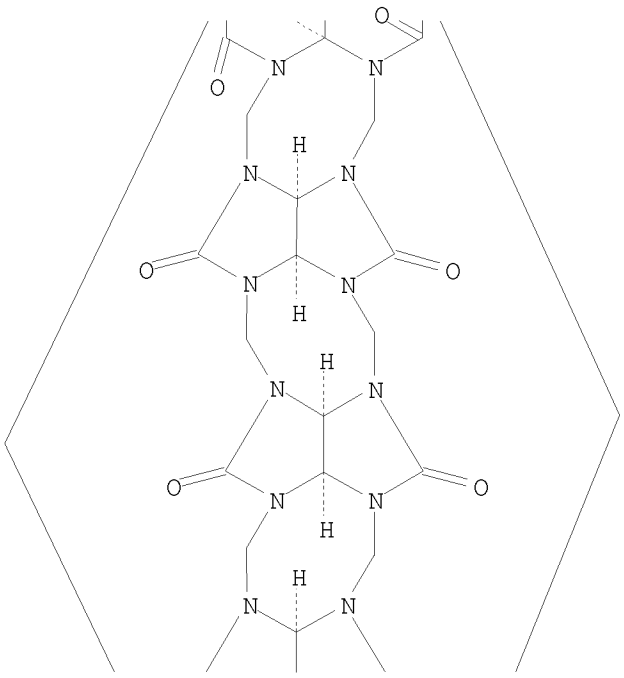
ntaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,22b-dimethyl-, stereoisomer
(CA INDEX NAME)

Relative stereochemistry.

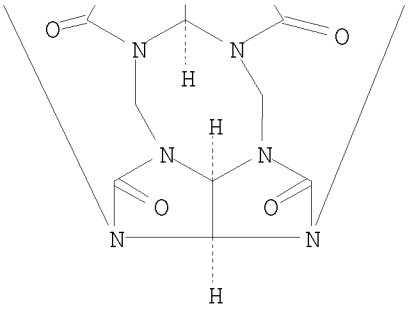
PAGE 1-A



PAGE 2-A



PAGE 3-A



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REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:851115 CAPLUS
DOCUMENT NUMBER: 149:246169
TITLE: Supramolecular assemblies based on some new methyl-substituted cucurbit[5]urils through hydrogen bonding
AUTHOR(S): Lu, Li-Bin; Yu, Da-Hai; Zhang, Yun-Qian; Zhu, Qian-Jiang; Xue, Sai-Feng; Tao, Zhu

CORPORATE SOURCE: Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Journal of Molecular Structure (2008), 885(1-3), 70-75
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:246169

AB Three supramol. assemblies based on three new partial methyl-substituted cucurbit[5]urils, which are tetramethylcucurbit[5]uril (α,γ-TMeQ[5]), hexamethyl cucurbit[5]uril (α,β,δ-HMeQ[5]), nonamethylcucurbit[5]uril (NMeQ[5]), were synthesized and structurally characterized by single-crystal X-ray diffractions. For the comparison with these new Q[5]s, crystal structure of an assembly constructing with normal Q[5] and K2PtCl6 was also reported. They are (α,γ-TMeQ[5])·15(H2O) (1), (α,β,δ-HMeQ[5])·2Cl-·2(H3O)+·7(H2O) (2), (NMeQ[5])·14(H2O) (3), (Q[5])2·[K(H2O)]2+·[PtCl6]2-·24(H2O) (4). In the corresponding crystal structures, the mol. encapsulates included a water mol. and lidded water mols. at both of the portals were observed Moreover, these mol. encapsulates are connected through hydrogen bonding and formed supramol. chains or joined in pair.

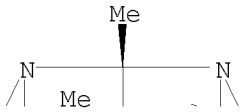
IT 1045861-31-1P 1045861-33-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystallog.; H-bonded supramol. assemblies based on methyl-substituted cucurbit[5]urils)

RN 1045861-31-1 CAPLUS

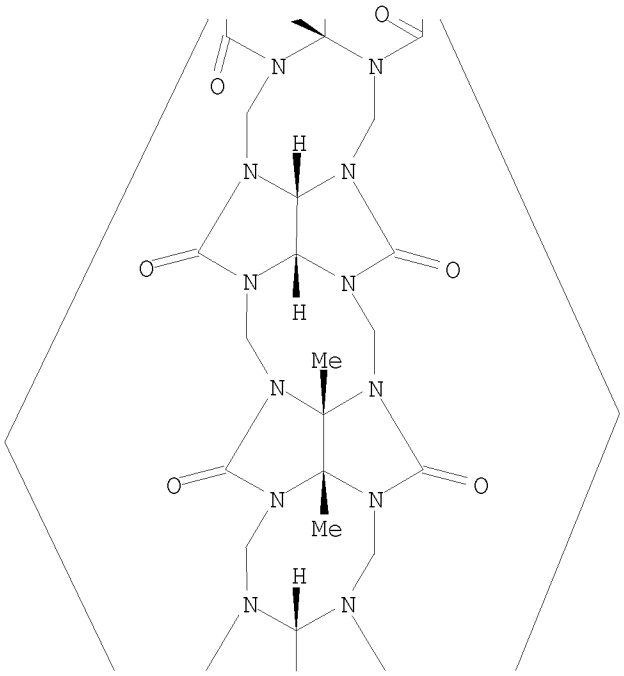
CN 1H,4H,12H,15H-2,14:3,13-Dimethano-5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,19b,19c,22b-tetramethyl-, hydrate (1:15), stereoisomer (CA INDEX NAME)

Relative stereochemistry.

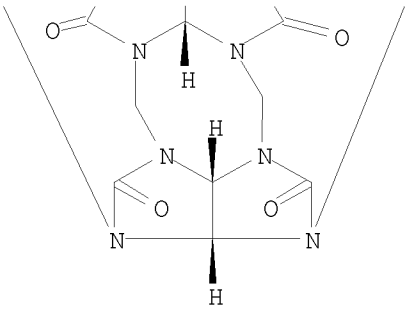
PAGE 1-A



PAGE 2-A



PAGE 3-A



●15 H_2O

RN 1045861-33-3 CAPLUS
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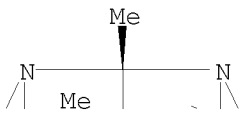
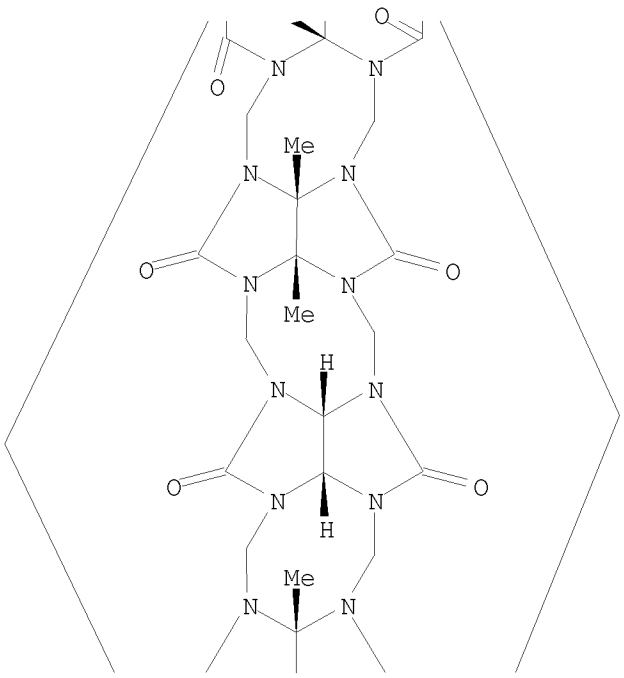
5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pe
ntaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,17b,17c,21b,21c,22b-
hexamethyl-, hydrochloride, hydrate (1:2:9), stereoisomer (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



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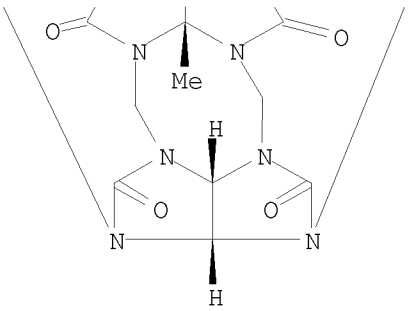


● 2 HCl

● 9 H_2O

OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:798206 CAPLUS
DOCUMENT NUMBER: 150:351448
TITLE: Host-guest Complex of a Water-soluble Cucurbit[6]uril Derivative with the Hydrochloride Salt of 3-amino-5-phenylpyrazole
AUTHOR(S): Feng, Yan; Xiao, Xin; Xue, Sai-Feng; Zhang, Yun-Qian; Zhu, Qian-Jiang; Tao, Zhu; Lawrance, Geoffrey A.; Wei, Gang
CORPORATE SOURCE: Institute of Applied Chemistry, Guizhou University, Guizhou, 550025, Peop. Rep. China
SOURCE: Supramolecular Chemistry (2008), 20(5), 517-525
CODEN: SCHEER; ISSN: 1061-0278
PUBLISHER: Taylor & Francis Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Interaction between tetramethylcucurbit[6]uril and 3-amino-5-phenylpyrazole hydrochloride in aqueous solution has been investigated by using 1H NMR spectroscopy, electronic absorption spectroscopy and fluorescence spectroscopy, as well as by a single crystal X-ray diffraction determination The 1H NMR spectra anal. established a basic interaction model in which an inclusion complex with a host:guest ratio of 1:1 forms, in which the host selectively binds the Ph moiety of the guest. Absorption spectrophotometric and fluorescence spectroscopic anal. in aqueous solution defined the stability of the host-guest inclusion complexes quant. as 6.8 + 105 mol- 1 L at pH 2.6; the interaction is pH dependent, decreasing as pH rises. The single crystal X-ray structure of the isolated inclusion complex shows the Ph moiety of the guest inserted into the host cavity, which supports particularly the 1H NMR spectroscopic study in solution In the crystal structure of the inclusion complex, the host-guest interaction involves both inter- and intra-complex hydrogen bonding, forming 2:2 dimers that stack in one dimension as supramol. tubes.
IT 1133166-99-0
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(crystal structure; host-guest complex of a water-soluble cucurbit[6]uril derivative with the hydrochloride salt of 3-amino-5-phenylpyrazole)
RN 1133166-99-0 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer, compd. with 5-phenyl-1H-imidazol-2-amine, hydrochloride, hydrate (1:1:1:14) (CA INDEX NAME)

CM 1

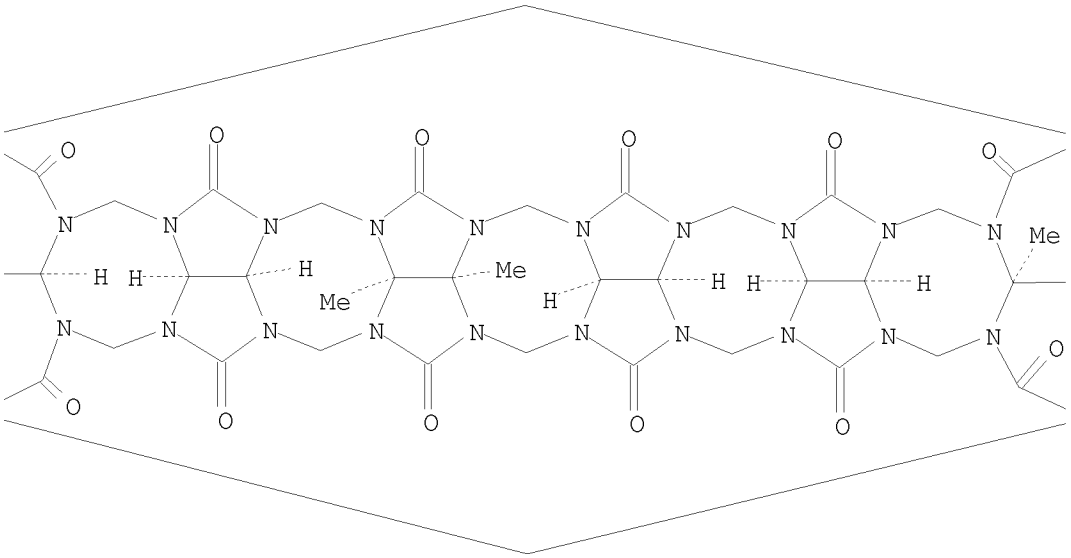
CRN 848440-56-2

CMF C40 H44 N24 O12

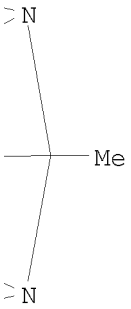
Relative stereochemistry.

PAGE 1-A

PAGE 1-B

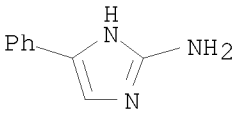


PAGE 1-C



CM 2

CRN 6775-40-2
CMF C9 H9 N3



IT 848440-56-2
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(host; host-guest complex of a water-soluble cucurbit[6]uril derivative with the hydrochloride salt of 3-amino-5-phenylpyrazole)

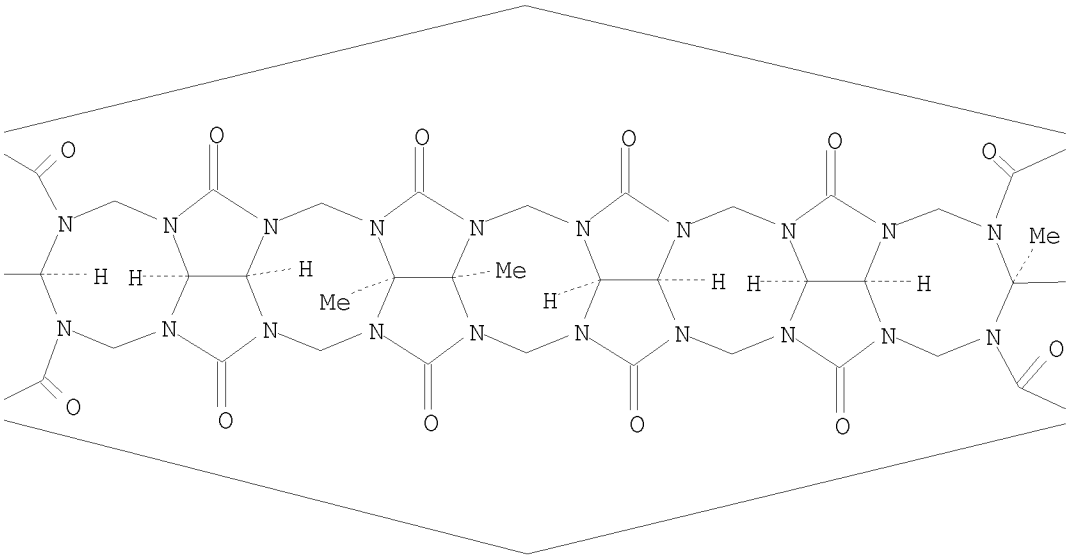
RN 848440-56-2 CAPLUS

CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

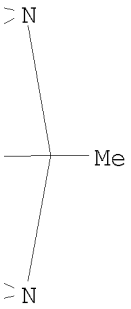
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:668053 CAPLUS
DOCUMENT NUMBER: 149:214504
TITLE: Structures of supramolecular assemblies formed by some partial substituted cucurbiturils and some metal ion complexes
AUTHOR(S): Yu, Da-Hai; Ni, Xin-Long; Zhang, Yun-Qian; Xue, Sai-Feng; Zhu, Qian-Jiang; Tao, Zhu
CORPORATE SOURCE: Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Journal of Molecular Structure (2008), 882(1-3), 128-133
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:214504
AB Three supramol. assemblies based on substituted cucurbit[6]uril, α,δ-tetramethylcucurbit[6]uril (TMeQ[6]), α,γ,ε-tricyclohexylcucurbit[6]uril (m-TriCyHQ[6]), and α,γ,ε-hexamethylcucurbit[6]uril (m-HMeQ[6]) with different metal ions were synthesized and structurally characterized by single-crystal x-ray diffractions. They are {TMeQ[6]@acetone[Ca(H2O)3]}2+·(CdCl4)2-·10H2O (1), {[m-TriCyHQ[6]@dioxane][Na(H2O)2Cl]}·15H2O (2) and {[m-HMeQ[6]]K2(H2O)4Cl}Cl·15H2O (3). The crystal structures of these complexes showed the different interaction modes between these partial alkyl-substituted cucurbit[6]urils and the metal ions. In compound 1, a 1-dimensional supramol. chain of alternating TMeQ[6] mols. and [Ca(H2O)3]2+ complexes assembled through coordination bonding of the cation and the carbonyl oxygens of TMeQ[6]. The compound 2 was the 1st

reported crystal structure of the m-TriCyHQ[6] with metal ion through the coordinate bonds, and the compound 3 was the 1st reported crystal structure of m-HMeQ[6]. It was unexpected that an ionic bonded chloride anion was at the portal of the two meta-substituted cucurbiturils.

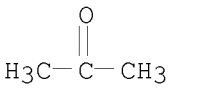
IT 1042142-05-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(one-dimensional chain polymer; preparation and crystal and mol. structure)

RN 1042142-05-1 CAPLUS

CN Calcium(2+), triaqua(dodecahydro-2a,21b,21c,26b-tetramethyl-1H,4H,14H,17H-2,16:3,15-dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cyclooocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone-κO1,κO17)-, (T-4)-tetrachlorocadmate(2-), compd. with 2-propanone, hydrate (1:1:1:10) (CA INDEX NAME)

CM 1

CRN 67-64-1
CMF C3 H6 O



CM 2

CRN 1042142-04-0
CMF C40 H50 Ca N24 O15 . Cd Cl4

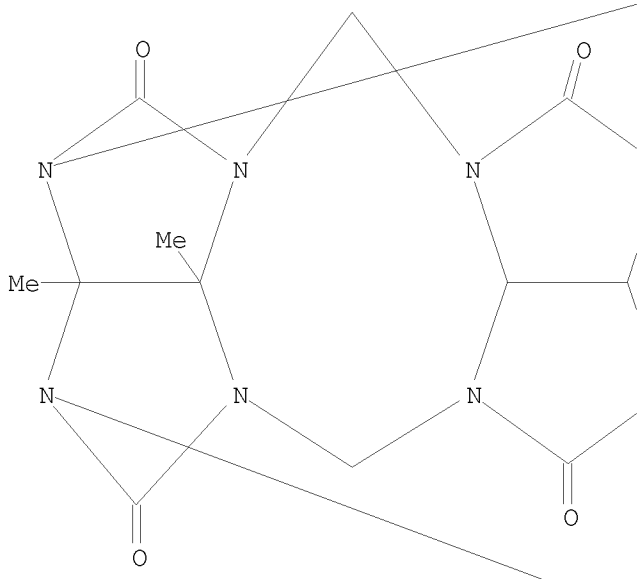
CM 3

CRN 1042142-03-9
CMF C40 H50 Ca N24 O15
CCI CCS

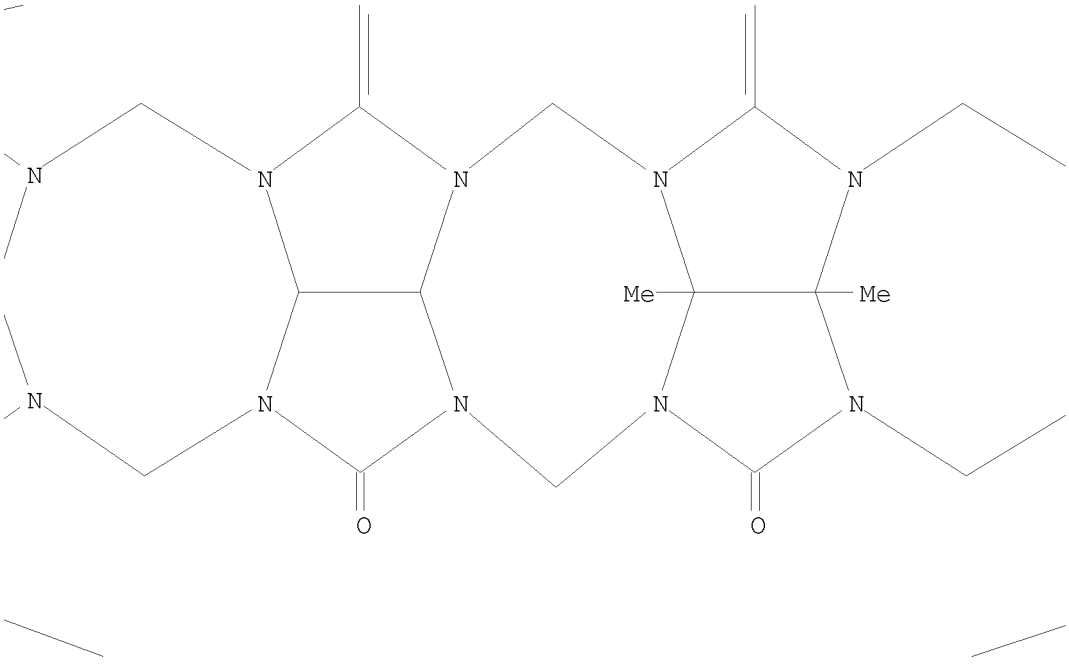
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

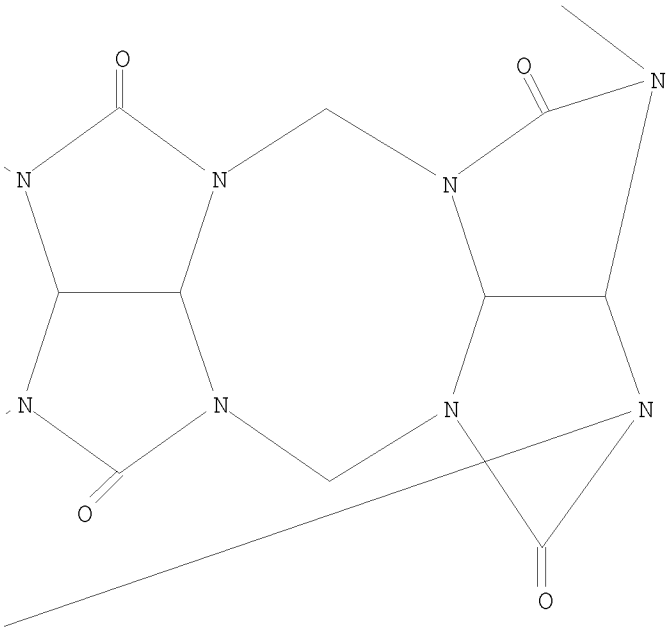
PAGE 2-A



PAGE 2-B



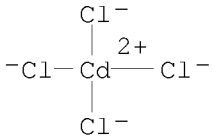
PAGE 2-C



PAGE 3-B

CM 4

CRN 15974-49-9
CMF Cd Cl4
CCI CCS

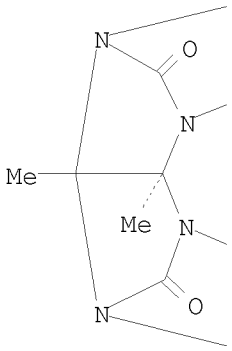


IT 640732-36-1 848440-56-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of calcium, sodium and potassium complexes with substituted cucurbit[6]urils)
RN 640732-36-1 CAPLUS

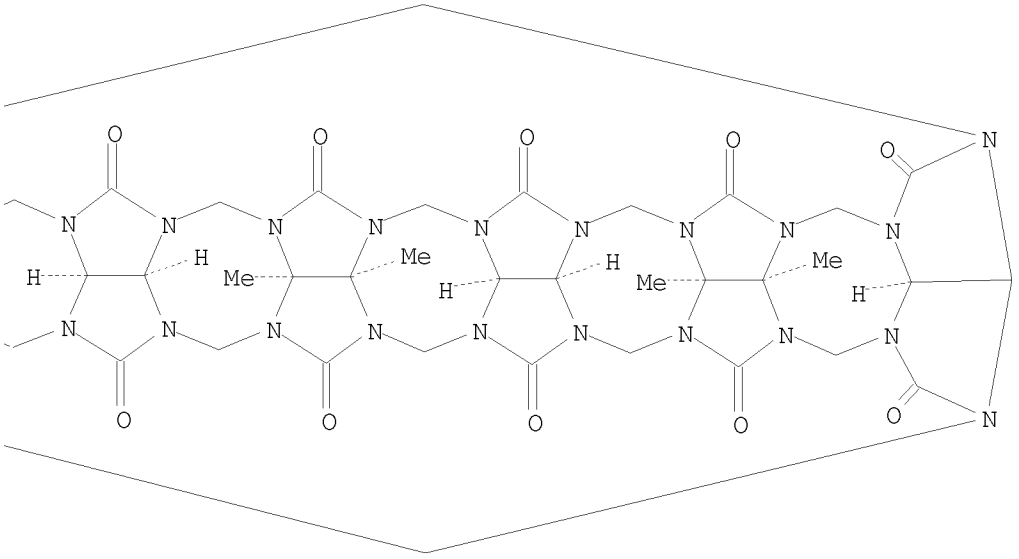
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,19b,19c,23b,23c,26b-hexamethyl-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



RN 848440-56-2 CAPLUS
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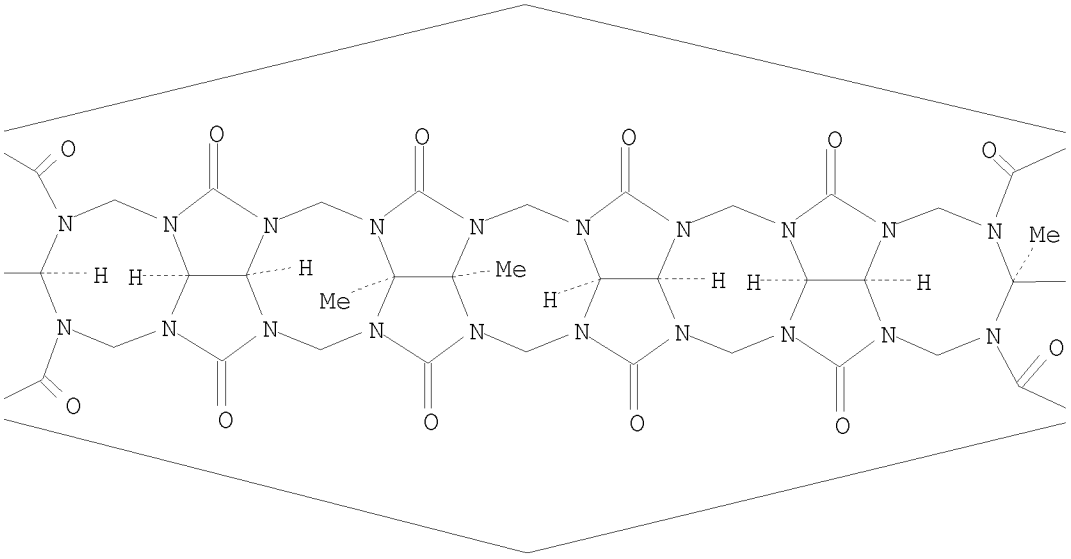
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

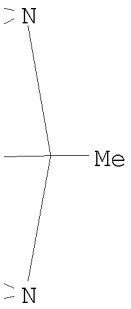
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:577915 CAPLUS
DOCUMENT NUMBER: 150:198924
TITLE: Solubility enhancement of kinetin through host-guest interactions with cucurbiturils
AUTHOR(S): Huang, Ying; Xue, Sai-Feng; Tao, Zhu; Zhu, Qian-Jiang; Zhang, Hong; Lin, Jing-Xiang; Yu, Da-Hai
CORPORATE SOURCE: Key Laboratory of Macrocyclic and Supramolecular Chemistry of Guizhou Province, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Journal of Inclusion Phenomena and Macrocyclic Chemistry (2008), 61(1-2), 171-177
CODEN: JIPCF5; ISSN: 1388-3127
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We explored the use of cucurbiturils to form inclusion complexes to overcome the solubility problems of kinetin, a plant cytokinin. Inclusion complexes between kinetin and Q[7], TMeQ[6] and HMeQ[6] in aqueous solution and in solid state were investigated by phase solubility studies, 1H NMR and IR. The effects of pH and temperature on complex stability were also investigated. Phase solubility studies showed that kinetin solubility increased in a linear fashion as a function of Q[7] and TMeQ[6] concns. However, kinetin solubility increased first, then decreased as the HMeQ[6] concentration increased, and the maximum solubility of kinetin was achieved at 4.95 mM in HMeQ[6]. The solubility of kinetin as well as the stability constant of its complex with Q[7] were affected by the pH of the medium. The thermodn. parameters of the complex formation were also determined, and it showed that the formation of the inclusion complexes between kinetin and Q[7] was enthalpy controlled,

suggesting that hydrophobic and van der Waals interactions were the main driving forces. Moreover, we found that the size of the cavity of cucurbituril played an important role in the association process. The formation of inclusion complexes between Q[7], TMeQ[6] and HMeQ[6] with kinetin was confirmed by 1H NMR, and IR spectroscopy showed the presence of inclusion complexes in solid state. Our results demonstrated that the complexation of kinetin with Q[n] could be used to improve the solubility of kinetin in aqueous solution

IT 848440-56-2
RL: PRP (Properties); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(solubility enhancement of kinetin through host-guest interactions with cucurbiturils)

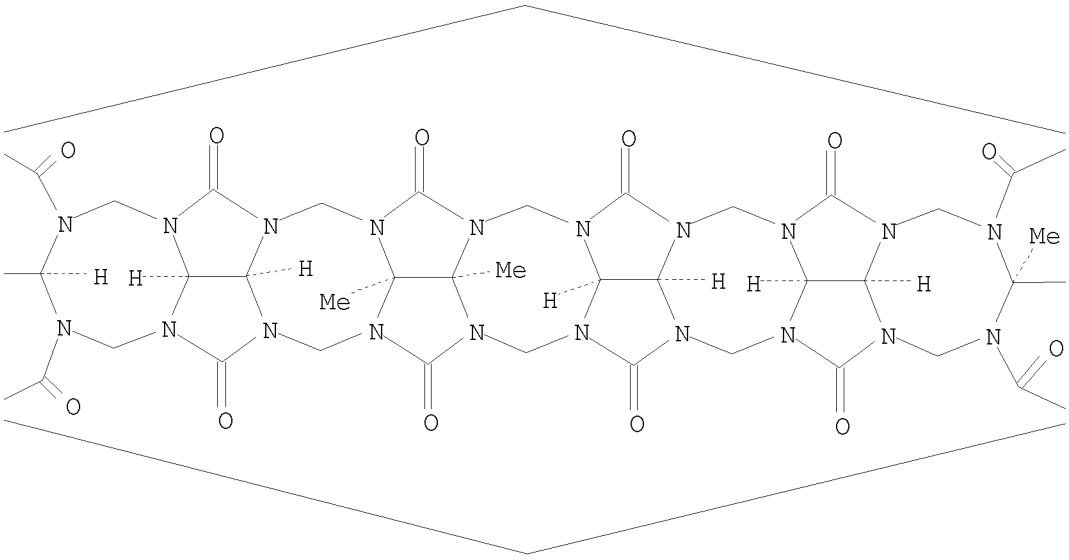
RN 848440-56-2 CAPLUS

CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

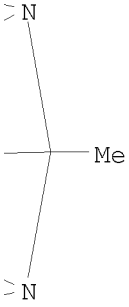
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



IT 1110783-33-9
RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(solubility enhancement of kinetin through host-guest interactions with cucurbiturils)

RN 1110783-33-9 CAPLUS

CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-

g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer, compd. with
N-(2-furanylmethyl)-9H-purin-6-amine (1:1) (CA INDEX NAME)

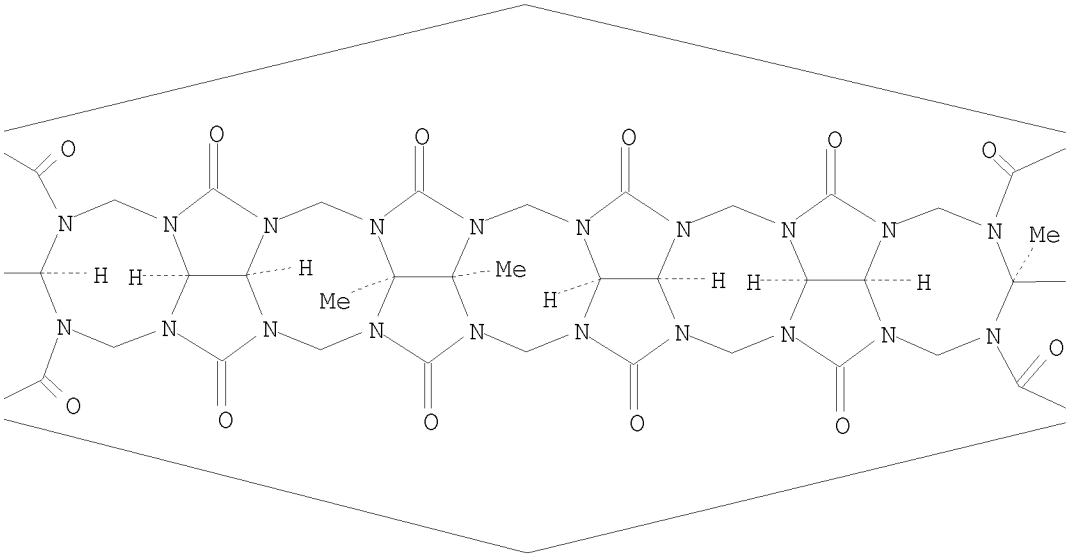
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

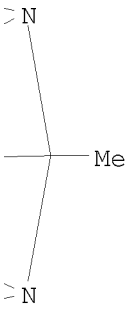
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



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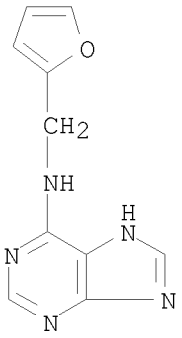
CRN 525-79-1
CMF C10 H9 N5 O



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 18 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:272306 CAPLUS
DOCUMENT NUMBER: 148:508829
TITLE: Structures of supramolecular assemblies formed by substituted cucurbiturils and metal ions
AUTHOR(S): Zhang, Yun-Qian; Zhen, Li-Mei; Yu, Da-Hai; Zhao, Yun-Jie; Xue, Sai-Feng; Zhu, Qian-Jiang; Tao, Zhu
CORPORATE SOURCE: Institute of Applied Chemistry, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Journal of Molecular Structure (2008), 875(1-3), 435-441

CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:508829

AB Four supramol. assemblies based on two partial substituted cucurbituril, α,δ-tetramethylcucurbit[6]uril (TMeQ[6]) and α,δ-dicyclohexanocucurbit[6]uril ((CyH)2Q[6]), with different metal ions were synthesized and structurally characterized by single-crystal x-ray diffractions. They are {[TMeQ[6]@2H2O].cntdot.[Zn(H2O)4]}·[ZnCl4]·12H2O (1), {[TMeQ[6]@H2O].cntdot.[Sr2Cl2]}.cntdot.[Cl]2.cntdot.10H2O (2), {TMeQ[6]·[CaCl]}·[Cl]·17.5H2O (3), {[(CyH)2Q[6]@acetone].cntdot.1.5[Ni(H2O)6]}·(NO3)32H2O (4). The crystal structures of these complexes showed that supramol. chains were formed through different interaction modes. In complex 1, the transition metal ion Zn2+ was coordinated not only with H2O mols. but also directly with carbonyl oxygens of a portal of TMeQ[6]. The Zn aqua complexes served as a bridge between TMeQ[6]s in the 1-dimensional supramol. chains. In complex 2, each Sr2+ ion was coordinated directly with two carbonyl O atoms at a portal of two TMeQ[6], and each TMeQ[6] was coordinated with four Sr2+ ions, giving supramol. chains consisted of alternating metal ions and TMeQ[6]. In 3, two TMeQ[6] mols. were coordinated by two Ca2+ ions to form a assembled unit. The assembled units were connected through H bonds, giving supramol. chains. In complex 4, supramol. chains consisted of alternating [Ni(H2O)]2+ complex cation and (CyH)2Q[6] were formed through H bonding.

IT 848440-56-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of zinc, strontium, calcium and nickel complexes with substituted cucurbiturils)

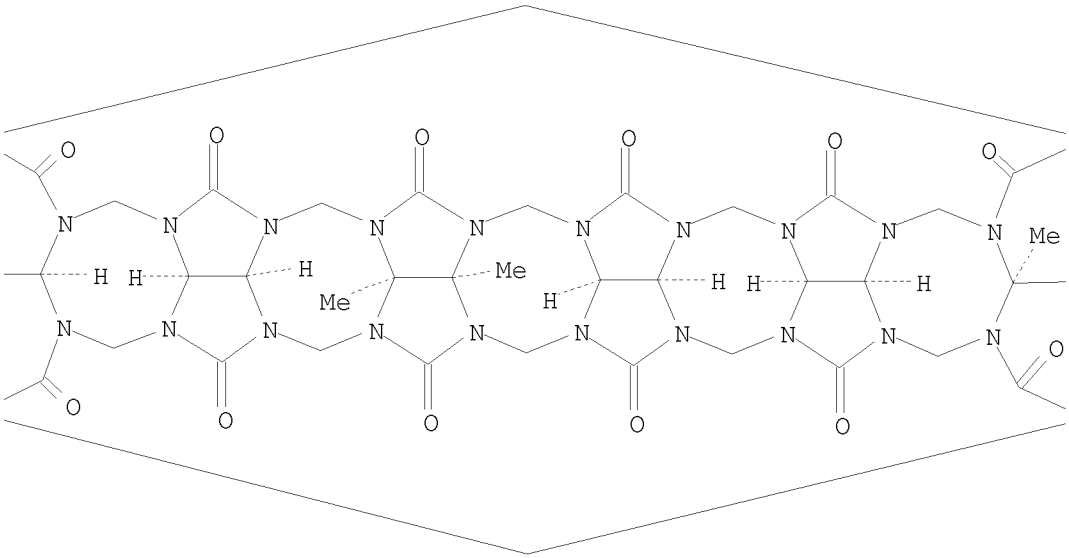
RN 848440-56-2 CAPLUS

CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

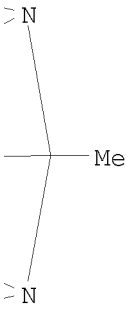
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C

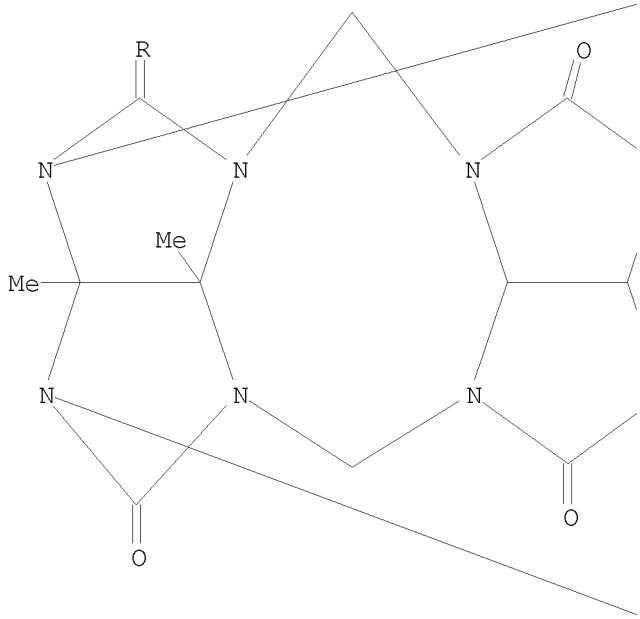


IT 1020725-95-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(polymeric; preparation and crystal structure of supramol. complex)
RN 1020725-95-4 CAPLUS
CN Strontium, hexaaquatetrachloro[μ-(dodecahydro-2a,21b,21c,26b-tetramethyl-1H,4H,14H,17H-2,16:3,15-dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone-κO1,κO17:κO21)]di-, hydrate (1:14) (CA INDEX NAME)

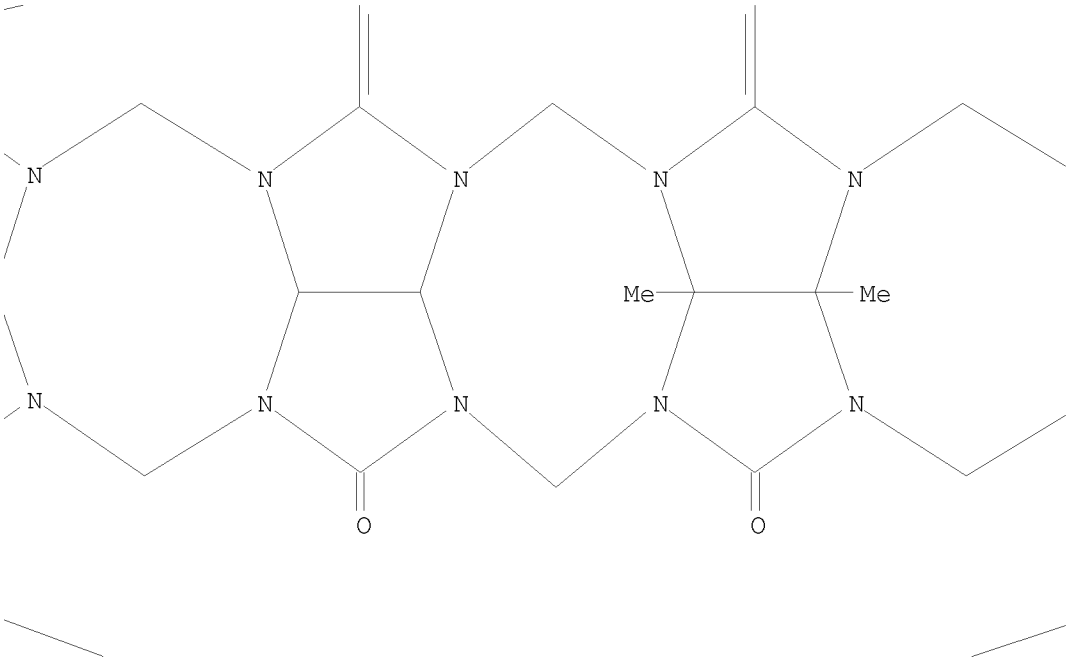
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

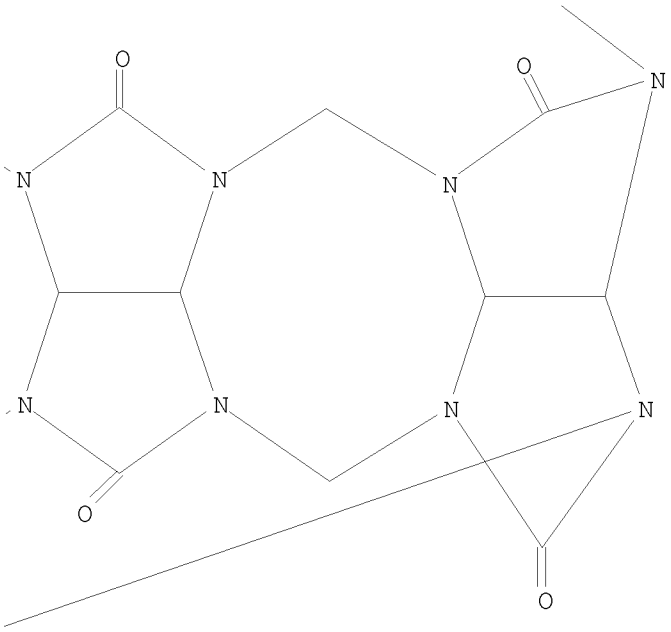
PAGE 2-A



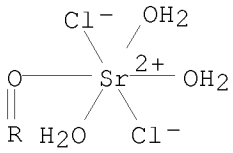
PAGE 2-B



PAGE 2-C



PAGE 3-A



●14 H_2O

PAGE 3-B

IT 1020725-94-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of supramol. complex)
RN 1020725-94-3 CAPLUS
CN Zinc(2+), tetraaqua(dodecahydro-2a,21b,21c,26b-tetramethyl-1H,4H,14H,17H-2,16:3,15-dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cyclooocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone-κO1,κO17)-, (OC-6-22)-, (T-4)-tetrachlorozincate(2-), hydrate (1:1:14) (CA INDEX NAME)

CM 1

CRN 1020725-93-2
CMF C40 H52 N24 O16 Zn . Cl4 Zn

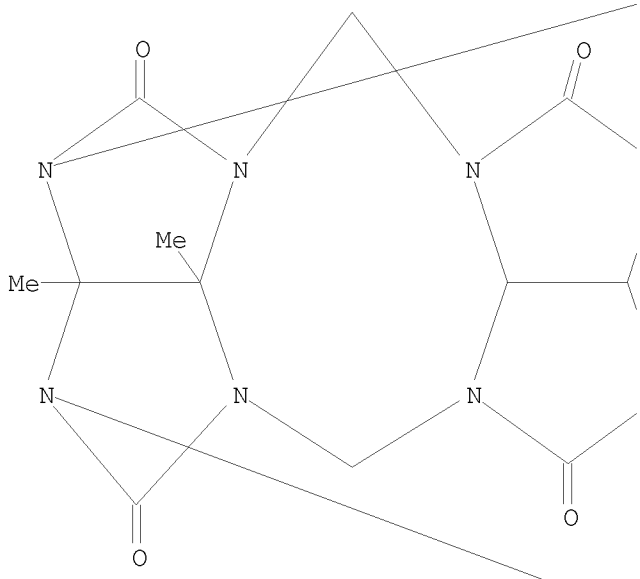
CM 2

CRN 1020725-92-1
CMF C40 H52 N24 O16 Zn
CCI CCS

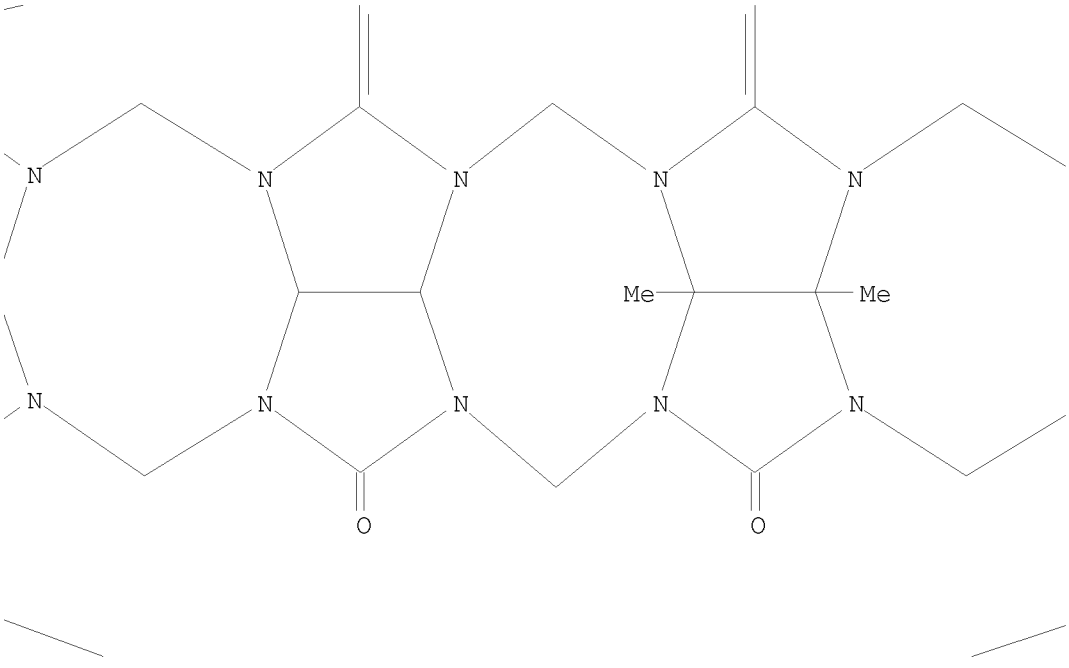
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

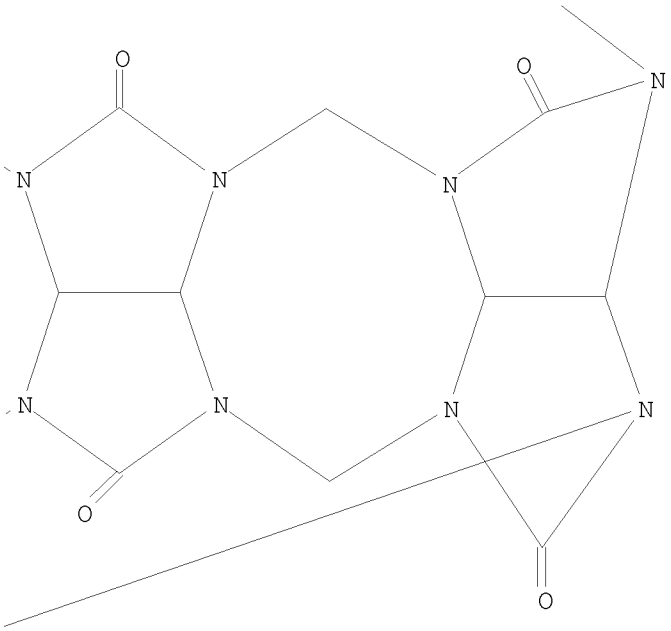
PAGE 2-A



PAGE 2-B



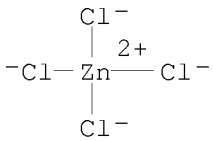
PAGE 2-C



PAGE 3-B

CM 3

CRN 15201-05-5
CMF Cl4 Zn
CCI CCS



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:111164 CAPLUS
DOCUMENT NUMBER: 148:262631
TITLE: Method for synthesis of cucurbit[n]urils and substituted cucurbit[n]urils compounds
INVENTOR(S): Xue, Saifeng; Zhu, Qianjiang; Tao, Zhu
PATENT ASSIGNEE(S): Guizhou University, Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 10pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 101108851	A	20080123	CN 2007-10077837	20070711
PRIORITY APPLN. INFO.:			CN 2007-10077837	20070711

AB The method comprises react glycoluril dimer with an epoxy glycoluril or an epoxy glycoluril derivative and formaldehyde in ratio 1:0-4:0-4 in hydrochloric acid at 90-100° for 1-2 h, concentrating, filtrating, separating and purifying to form cucurbit[n]urils or substituted cucurbit[n]urils, wherein the content of epoxy glycoluril or its derivative and formaldehyde is not simultaneously 0. The formaldehyde can be replaced by hexamethylenetetramine or polyformaldehyde; HCl can be replaced by sulfuric acid. With the method, the distribution of cucurbit[n]urils in product and the amount and position of substations groups in cucurbit[n]urils can be easily controlled.

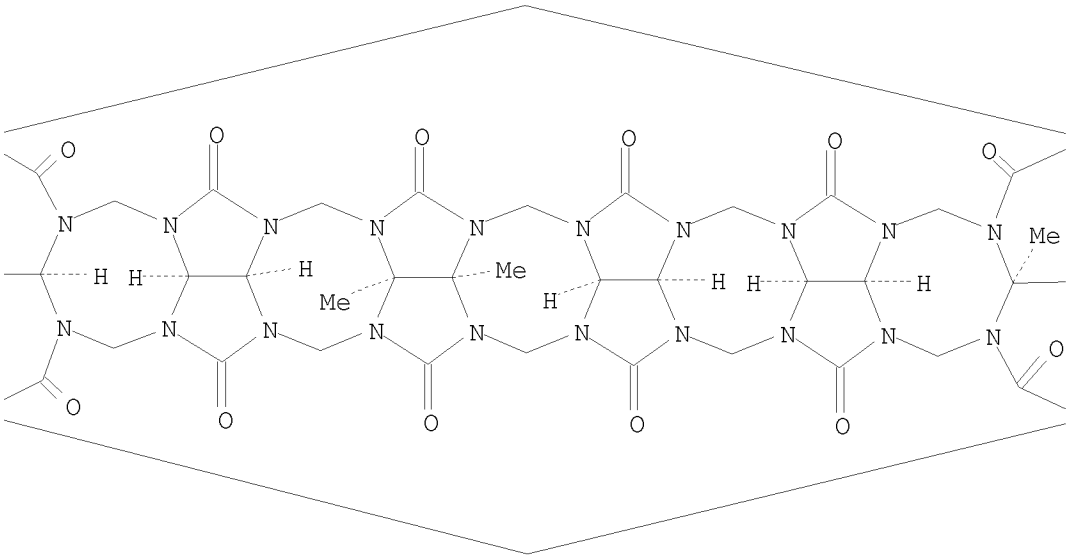
IT 848440-56-2P
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(method for synthesis of cucurbit[n]urils and substituted cucurbit[n]urils compds.)

RN 848440-56-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

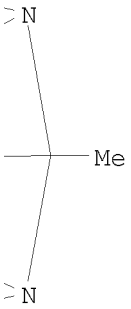
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



L4 ANSWER 20 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2007:1339803 CAPLUS
DOCUMENT NUMBER: 148:561422
TITLE: Studies of the interaction of tetramethylcucurbit[6]uril and 5,5'-dimethyl-2,2'-bipyridyl hydrochloride
AUTHOR(S): Cong, Hang; Zhao, Yun-Jie; Xue, Sai-Feng; Tao, Zhu; Zhu, Qian-Jiang
CORPORATE SOURCE: Institute of Applied Chemistry, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Journal of Molecular Modeling (2007), 13(12), 1221-1226
CODEN: JMMOFK; ISSN: 0948-5023
URL: http://www.springerlink.com/content/x6nw1j3949222664/fulltext.pdf
PUBLISHER: Springer GmbH
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
AB The interaction between tetramethylcucurbit[6]uril (host) and 5,5'-dimethyl-2,2'-bipyridyl hydrochloride (guest) was studied by 1H NMR, x-ray crystallog., electronic absorption spectroscopy, fluorescence emission spectra and quantum chemical calcns. This exptl.-computational study that indicated the host can orientationally encapsulate the guest with a moderate association constant value. Computation qual. explained the split UV-visible absorption peak of the inclusion complex.
IT 1026700-36-6
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)
(interaction of tetramethylcucurbit[6]uril host and 5,5'-dimethyl-2,2'-bipyridyl hydrochloride guest)
RN 1026700-36-6 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2''

,3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer, compd. with 5,5'-dimethyl-2,2'-bipyridine hydrochloride, hydrate (1:1:1:?) (CA INDEX NAME)

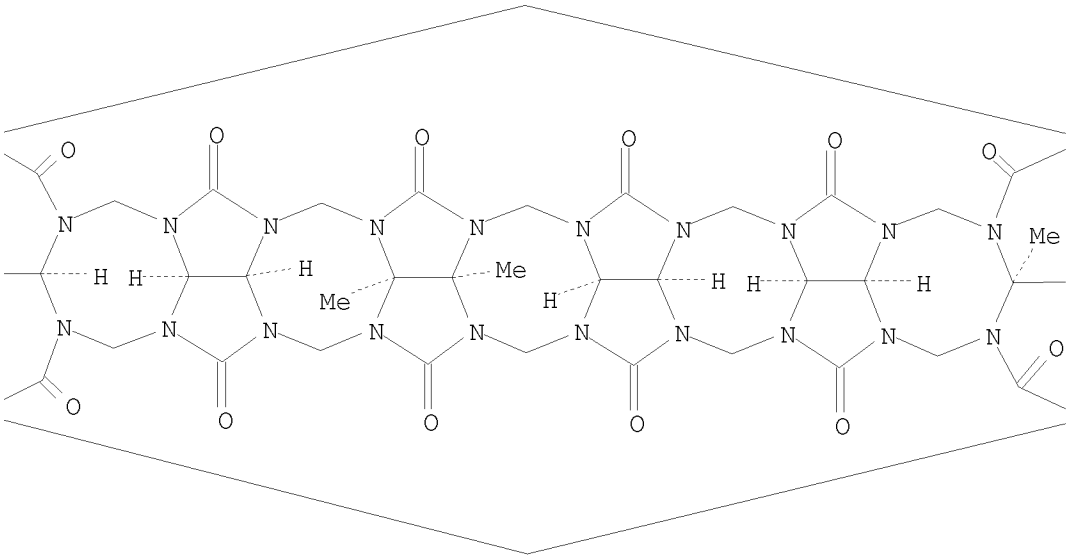
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

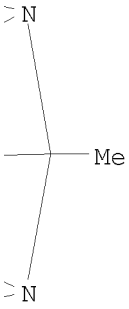
Relative stereochemistry.

PAGE 1-A

PAGE 1-B

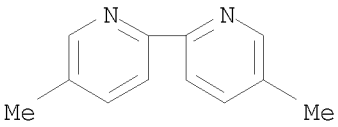


PAGE 1-C



CM 2

CRN 1762-34-1
CMF C12 H12 N2

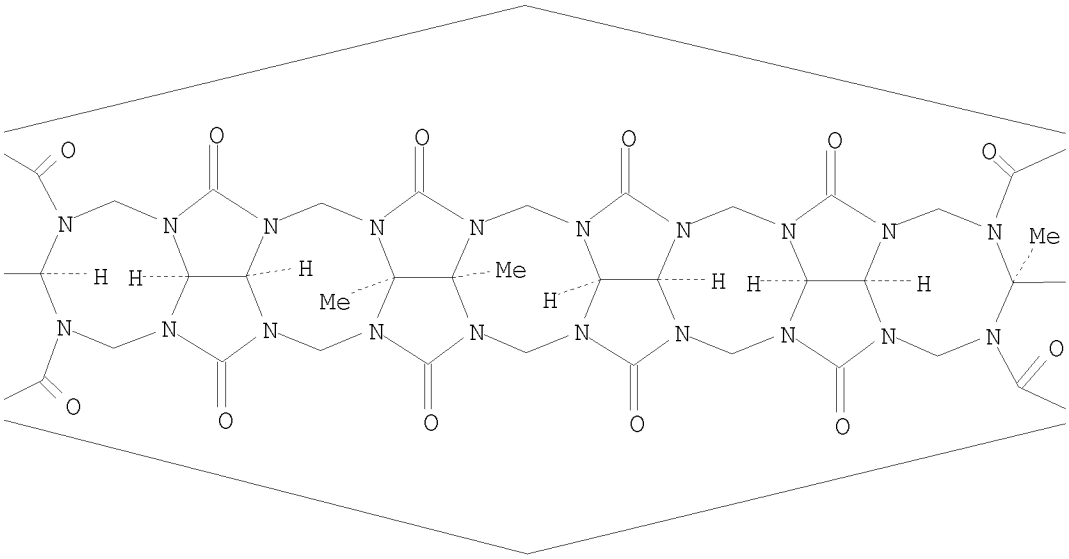


IT 848440-56-2
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(interaction of tetramethylcucurbit[6]uril host and 5,5'-dimethyl-2,2'-bipyridyl hydrochloride guest)
RN 848440-56-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

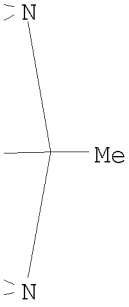
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 21 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2007:508326 CAPLUS
DOCUMENT NUMBER: 147:165907
TITLE: Synthesis and X-ray structure of the inclusion complex of dodecamethylcucurbit[6]uril with 1,4-dihydroxybenzene
AUTHOR(S): Lu, Li-Bin; Zhang, Yun-Qian; Zhu, Qian-Jiang; Xue, Sai-Feng; Tao, Zhu

CORPORATE SOURCE: Institute of Applied Chemistry, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Molecules (2007), 12(4), 716-722
CODEN: MOLEFW; ISSN: 1420-3049
URL: http://www.mdpi.org/molecules/papers/12040716.pdf
PUBLISHER: Molecular Diversity Preservation International
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:165907

AB The synthesis, and x-ray crystal structure of the inclusion host-guest complex of dodecamethylcucurbit[6]uril (DDMeQ[6]) with 1,4-dihydroxybenzene (DHOBEN) are reported. The complex crystallizes in the space group P21/c with a = 12.2847(4), b = 12.6895(4), c = 15.1310(4) Å, α = 74.6960(10), β = 71.4090(10), γ = 86.5090(10)° and Z = 1. A novel approach to dodecamethylcucurbit[6]uril synthesis is also described. To sep. dodecamethylcucurbit[6]uril, 1,4-dihydroxybenzene is used as a guest mol. for crystallization of the fully methyl-substituted cucurbituril. The driving force for the self-assembled inclusion host-guest complex can be attributed to not only the cavity interaction of dodecamethylcucurbit[6]uril (host), but also to the hydrogen bonding between the carbonyl oxygen at the portals of the host and the hydroxy groups of the guest.

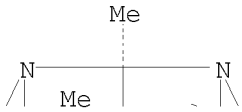
IT 569359-77-9
RL: PRP (Properties)
(preparation and X-ray structure of inclusion complex of dodecamethylcucurbit[6]uril with 1,4-dihydroxybenzene)

RN 569359-77-9 CAPLUS

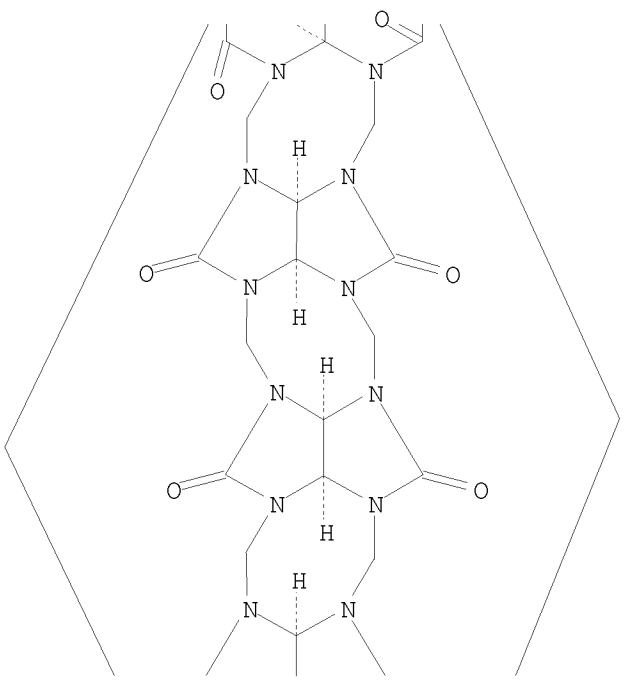
CN 1H,4H,12H,15H-2,14:3,13-Dimethano-5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,22b-dimethyl-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

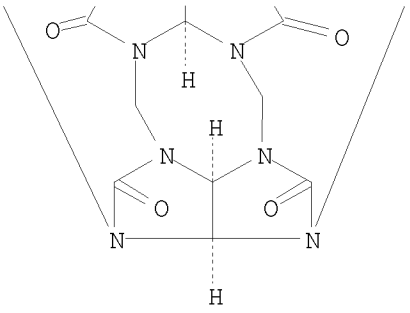
PAGE 1-A



PAGE 2-A



PAGE 3-A



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 22 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2007:408339 CAPLUS
DOCUMENT NUMBER: 147:52550
TITLE: Interaction between Tetramethylcucurbit[6]uril and Some Pyridine Derivates
AUTHOR(S): Cong, Hang; Tao, Long-Ling; Yu, Yi-Hua; Tao, Zhu; Yang, Fan; Zhao, Yun-Jie; Xue, Sai-Feng; Lawrance, Geoffrey A.; Wei, Gang
CORPORATE SOURCE: Institute of Applied Chemistry, Guizhou University, Guiyang, Guizhou, 550025, Peop. Rep. China
SOURCE: Journal of Physical Chemistry A (2007), 111(14), 2715-2721
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Interaction between tetramethylcucurbit[6]uril (TMeQ[6], host) with hydrochloride salts of 2-phenylpridine (G1), 2-benzylpyridine (G2), and 4-benzylpyridine (G3) (guests) have been investigated by using 1H NMR spectroscopy and electronic absorption spectroscopy and theor. calcns. The 1H NMR spectra anal. established an interaction model in which the host selectively included the Ph moiety of the HCl salt of the above three guests, and formed inclusion complexes with a host-guest ratio of 1:1. Absorption spectrophotometric anal. allowed quant. measurement of the stability of these host-guest inclusion complexes. Particularly, we have established a competitive interaction in which one host-guest inclusion complex pair is much more stable than another host-guest inclusion complex pair. The stability consts. for the three host-guest inclusion complexes of TMeQ[6]-G1, TMeQ[6]-G2, and TMeQ[6]-G3 are .apprx.2 + 106, 60.7, and 19.9 mol-1·L, resp. To understand how subtle differences in the structure of the title guests lead to a significant difference in the stability of the corresponding host-guest inclusion complexes with the TMeQ[6], ab initio theor. calcns. have been performed, not only for the gas phase but also the solution phase (water as solvent) in all cases. The calcn. results revealed that when the Ph moiety of the three pyridine derivate guests was included, the host-guest complexation reached the

min., and the corresponding energy differences for the formation of the title host-guest inclusion complexes are qual. consistent with the exptl. results.

IT 848440-56-2 939823-44-6 939823-46-8
939823-48-0
RL: PRP (Properties)
(interaction between tetramethylcucurbit[6]uril and some pyridine derivates)

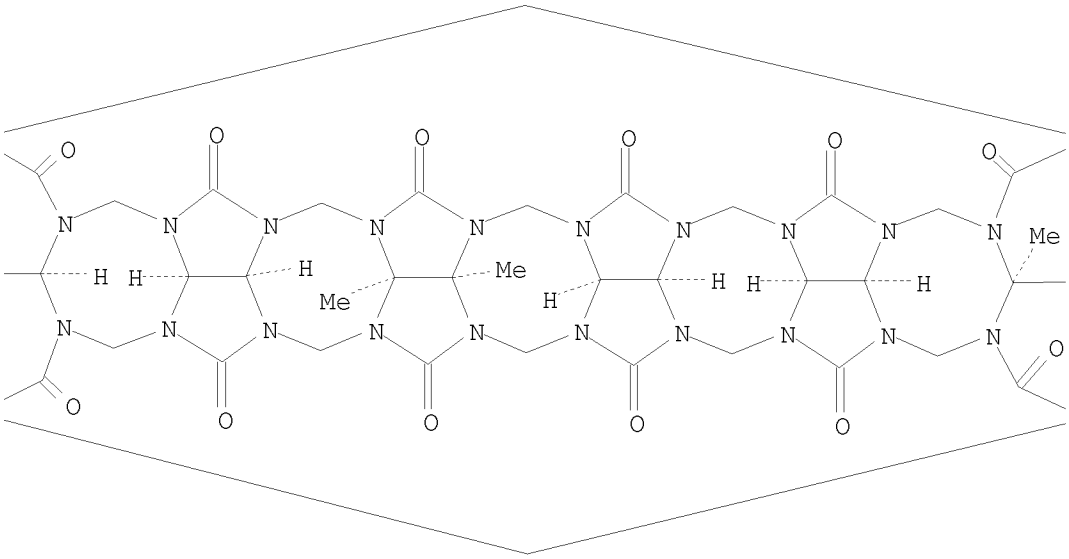
RN 848440-56-2 CAPLUS

CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

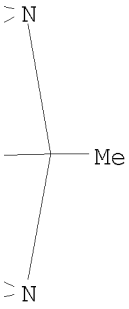
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



RN 939823-44-6 CAPLUS
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2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24
a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2''
,3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-
g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer, compd. with
2-phenylpyridine (2:5) (CA INDEX NAME)

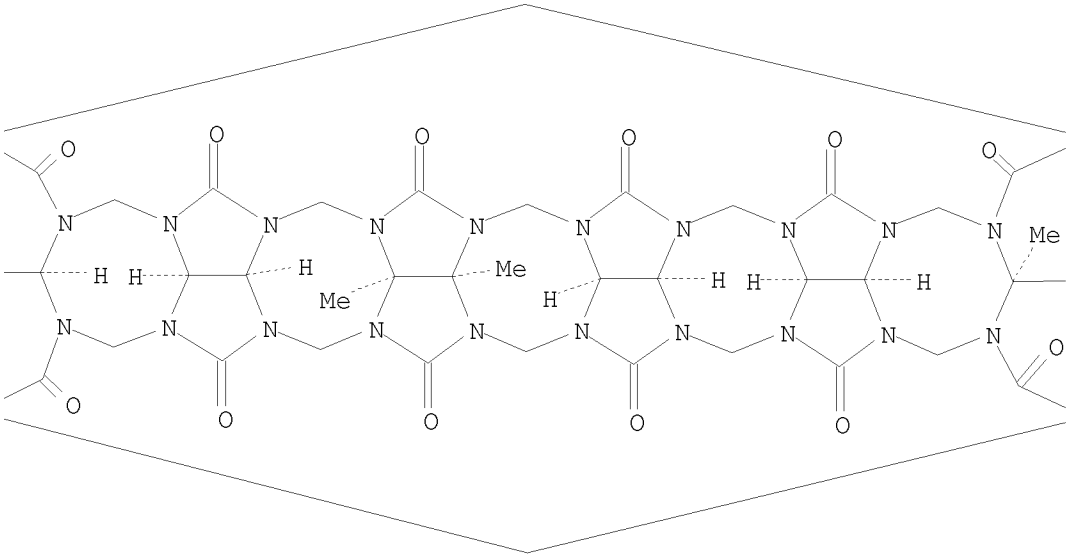
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

Relative stereochemistry.

PAGE 1-A

PAGE 1-B



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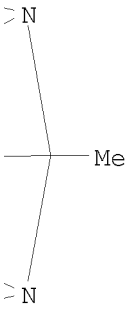

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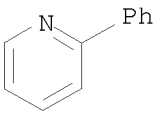
CRN 1008-89-5
CMF C11 H9 N



RN 939823-46-8 CAPLUS
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5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer, compd. with
2-(phenylmethyl)pyridine (2:5) (CA INDEX NAME)

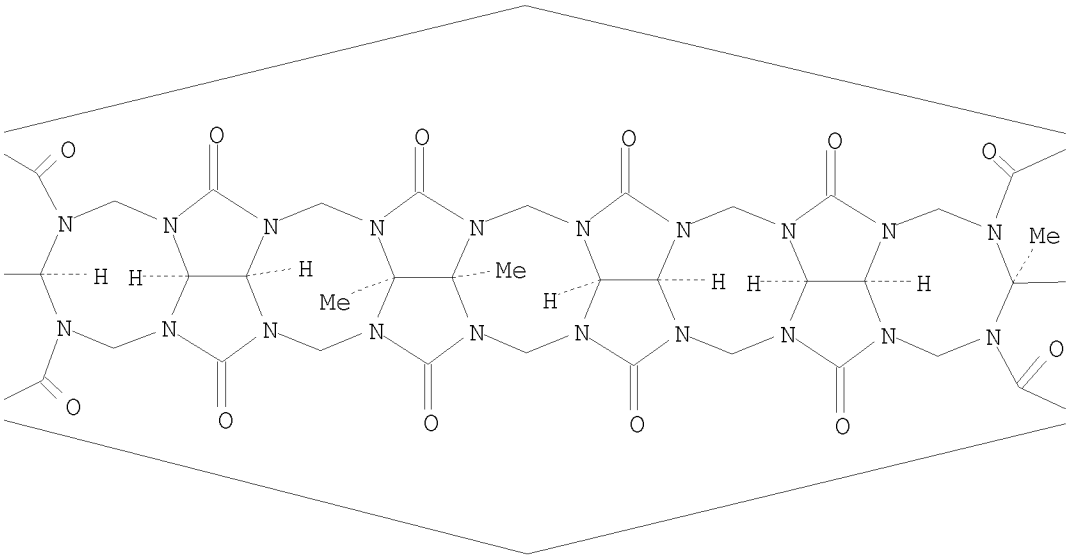
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

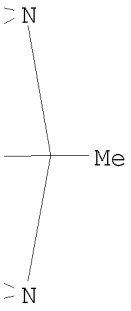
Relative stereochemistry.

PAGE 1-A

PAGE 1-B

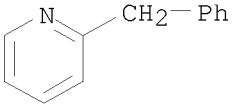


PAGE 1-C



CM 2

CRN 101-82-6
CMF C12 H11 N



RN 939823-48-0 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer, compd. with
4-(phenylmethyl)pyridine (2:5) (CA INDEX NAME)

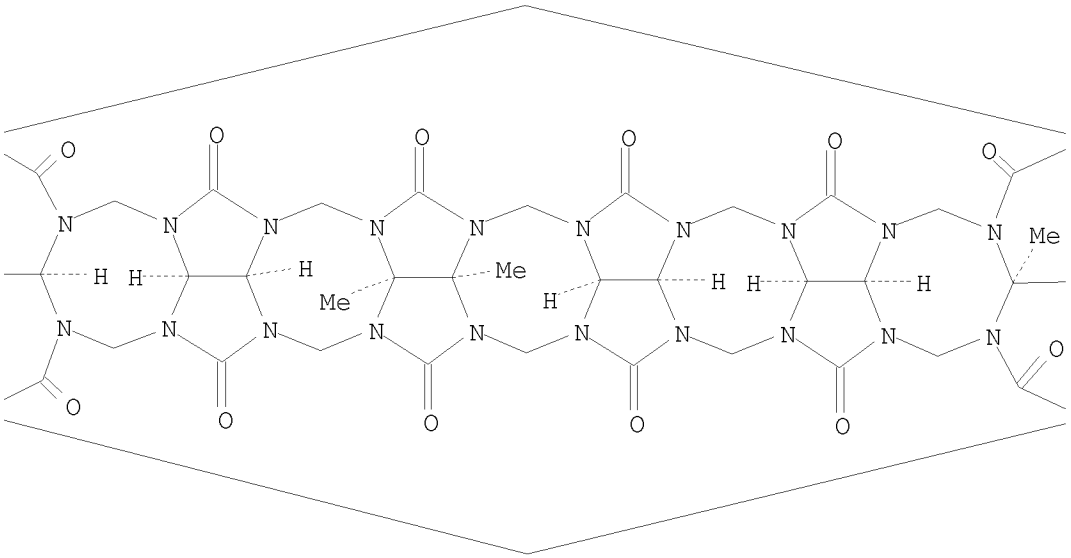
CM 1

CRN 848440-56-2
CMF C40 H44 N24 O12

Relative stereochemistry.

PAGE 1-A

PAGE 1-B



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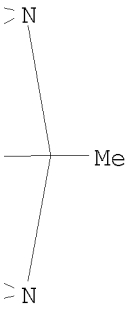
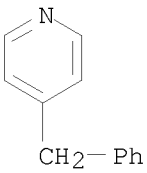


CM 2

CRN 2116-65-6
CMF C12 H11 N



OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 23 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2006:404036 CAPLUS
DOCUMENT NUMBER: 144:450383
TITLE: Interaction between three cucurbiturils and hydrochloride salts of 4,4'-dipyridyl and its derivates
AUTHOR(S): Mu, Lan; Xue, Sai-Feng; Du, Ying; Zhao, Yun-Jie; Zhu, Qian-Jiang; Tao, Zhu
CORPORATE SOURCE: Inst. Appl. Chem., Guizhou Univ., Guiyang, 550025, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (2006), 27(4), 654-659
CODEN: KTHPDM; ISSN: 0251-0790
PUBLISHER: Gaodeng Jiaoyu Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB In this paper, the host-guest relationship between a general cucurbit[n = 7]uril(Q[7]) or a new ellipsoid-host - sym. tetramethyl-cucurbituril

(TMeQ[6]) with hydrochloride salts of 4,4'-dipyridyl(44) or N,N'-dimethyl-4,4'-dipyridyl(dm44) was examined for confirming the interaction between cucurbituril(Q[6]) and these guests. The exptl. results revealed that Q[7] included the 4,4'-dipyridyl part of this kind of guests which were inclined in the cavity of Q[7]. The results based on 1H NMR technique, cyclic voltammetric method and UV absorption spectrophotometric measurement revealed that strong interaction existed between TMeQ[6] and guest 44 or dm44 and a one-dimensional assembled superamol. could be formed. 1H NMR technique and cyclic voltammetric method showed no obvious interaction between Q[6] with the guest 44 and its derivative, however, UV absorption spectrophotometric measurements revealed that a kind of interaction did occur; comparing the structural characteristic of Q[6] to TMeQ[6], a one-dimensional assembled superamol. could be also formed between Q[6] and guest 44 and its derivative

IT 848440-56-2
RL: PRP (Properties)
(interaction between three cucurbiturils and hydrochloride salts of 4,4'-dipyridyl and N,N'-dimethyl-4,4'-dipyridinium)

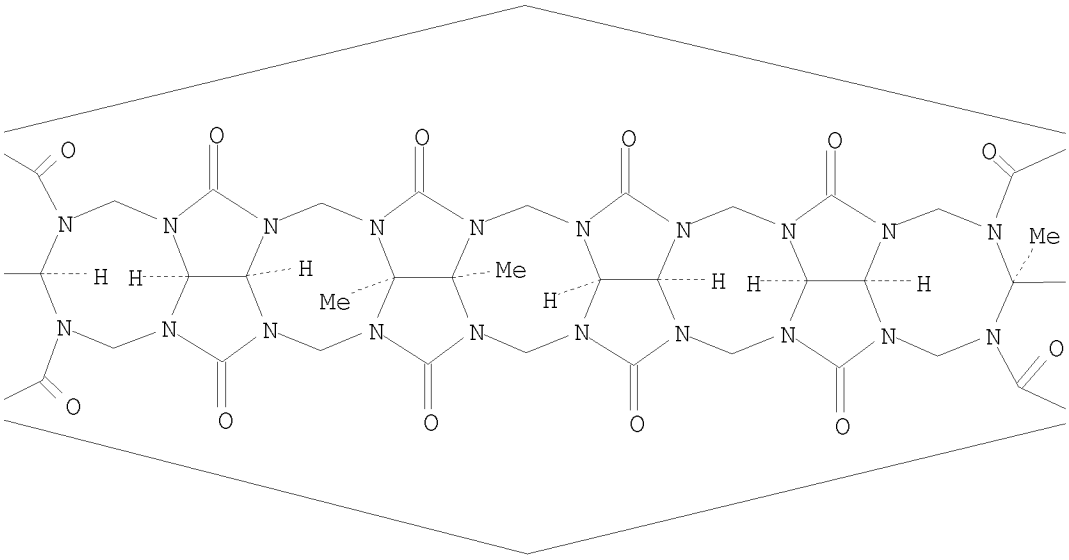
RN 848440-56-2 CAPLUS

CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

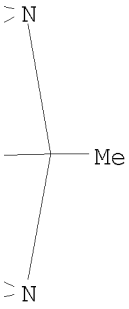
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L4 ANSWER 24 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:1142893 CAPLUS
DOCUMENT NUMBER: 144:323501
TITLE: Synthesis and crystal structure of a novel self-assembled 1,4-dimethyl cucurbituril silver(I) complex
AUTHOR(S): Zhang, Yun-Qian; Tao, Zhu; Zhao, Yun-Jie; Xue, Sai-Feng; Zhu, Qian-Jiang; Wei, Zhan-Bing; Long,

La-Sheng
CORPORATE SOURCE: Institute of Applied Chemistry, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Wuji Huaxue Xuebao (2005), 21(10), 1576-1582
CODEN: WHUXEO; ISSN: 1001-4861
PUBLISHER: Wuji Huaxue Xuebao Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 144:323501
AB Crystals of a new 1,4-di-Me cucurbituril (TMeQ [6]) with Silver(I) ion were synthesized, and the structure was determined by X-ray diffraction technique. There are two kinds of TMeQ[6] A and B which formed mol. encapsulates with two silver ion lids in the self-assembled entities. One dimensional supramol. tubes are formed from the encapsulates A, and two dimensional mol. sieves are formed from the encapsulates B, the tubes and the sieves stack together alternately in the self-assembled entities.
IT 880076-32-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of a novel self-assembled 1,4-di-Me cucurbituril silver(I) complex)
RN 880076-32-4 CAPLUS
CN Silver(2+), diaqua(dodecahydro-2a,21b,21c,26b-tetramethyl-1H,4H,14H,17H-2,16:3,15-dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone)di-, tetraaqua(dodecahydro-2a,21b,21c,26b-tetramethyl-1H,4H,14H,17H-2,16:3,15-dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone)disilver(2+) nitrate (1:1:4), octahydrate (9CI) (CA INDEX NAME)

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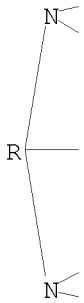
CRN 880076-31-3
CMF C40 H52 Ag2 N24 O16 . C40 H48 Ag2 N24 O14 . 4 N O3

CM 2

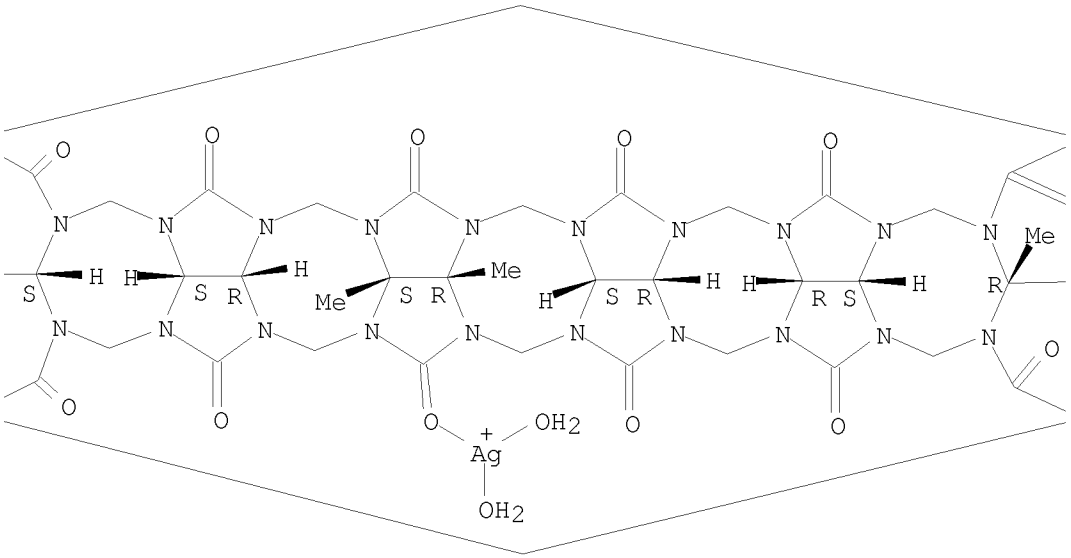
CRN 880076-30-2
CMF C40 H52 Ag2 N24 O16
CCI CCS

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



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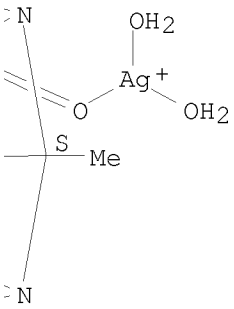
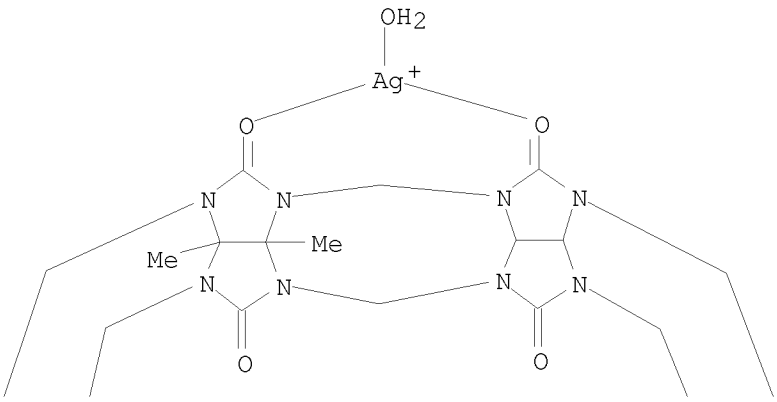


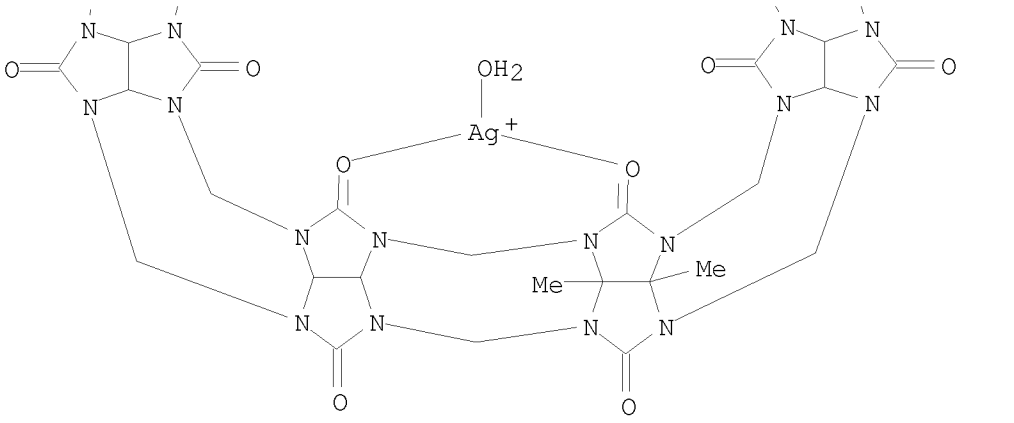
CM 3

CRN 880076-29-9
CMF C40 H48 Ag2 N24 O14
CCI CCS

PAGE 1-A

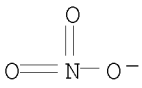


PAGE 2-A



CM 4

CRN 14797-55-8
CMF N O3

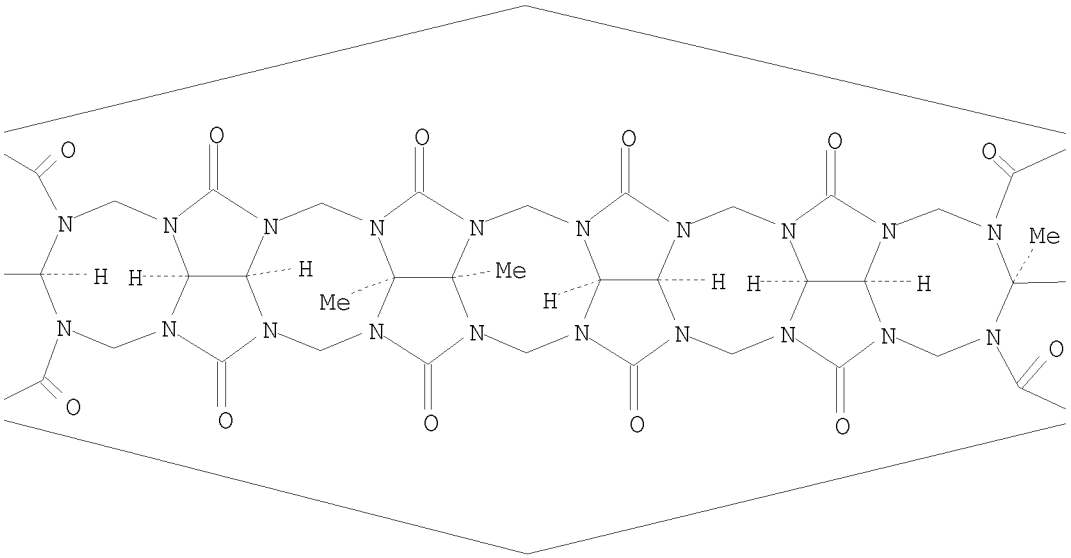


IT 848440-56-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of a novel self-assembled 1,4-di-Me cucurbituril silver(I) complex)
RN 848440-56-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

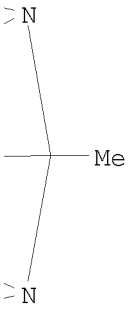
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



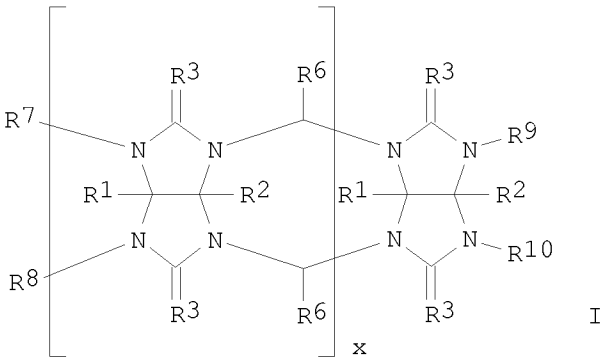
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L4 ANSWER 25 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:1042246 CAPLUS
DOCUMENT NUMBER: 143:347171
TITLE: Method for preparing compounds comprising cucurbituril groups
INVENTOR(S): Day, Anthony Ivan
PATENT ASSIGNEE(S): Unisearch Limited, Australia
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005090351	A1	20050929	WO 2005-AU396	20050318
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005222730	A1	20050929	AU 2005-222730	20050318
CA 2556857	A1	20050929	CA 2005-2556857	20050318
EP 1725558	A1	20061129	EP 2005-714268	20050318
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
CN 1930169	A	20070314	CN 2005-80007986	20050318

JP 2007529428	T	20071025	JP 2007-503155		20050318
IN 2006DN04501	A	20070824	IN 2006-DN4501		20060803
KR 2006135775	A	20061229	KR 2006-717057		20060824
US 20070287836	A1	20071213	US 2007-588846		20070430
PRIORITY APPLN. INFO.:			AU 2004-901473	A	20040319
			WO 2005-AU396	W	20050318

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 143:347171; MARPAT 143:347171
GI



I

AB The present invention provides a method for preparing compds. comprising a plurality of cucurbituril groups. The method comprises forming a mixture comprising one or more compds. of the formula A-L-A wherein L is a linking group and A is group of the formula I [R1 and R2 independently = bond with L or univalent radical, or R1,R2 and the carbon atoms to which they are bound together from an (un)substituted cyclic group, or R1 of one unit and R2 of adjacent unit from a bond or divalent radical, etc.; R3 = O, S, NH, etc.; R6 = bond with L, H, alkyl, and aryl; R7 and R8 or R9 and R10 independently = H and CHR6OR6, or R7 and R8 together form the group -CHR6OCHR6-; x = 0-10 with provisions], and an acid, and exposing the mixture to conditions effective for at least some of the groups A to form cucurbituril groups.

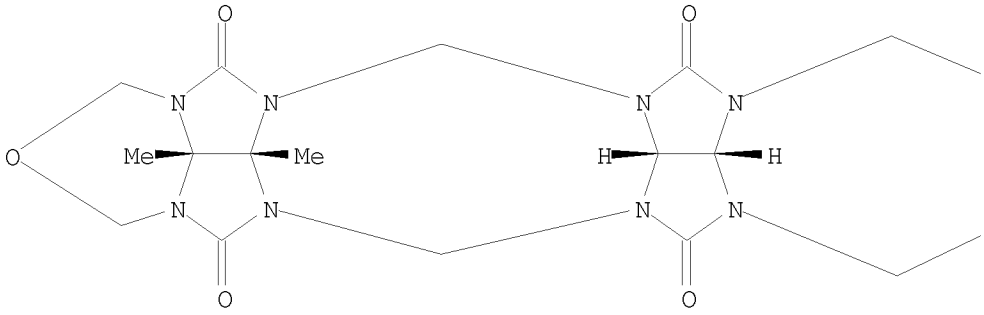
IT 865813-91-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of dimer, trimer and tetramers of glycolurils useful for preparing
compound containing plurality of cucurbituril groups)

RN 865813-91-8 CAPLUS

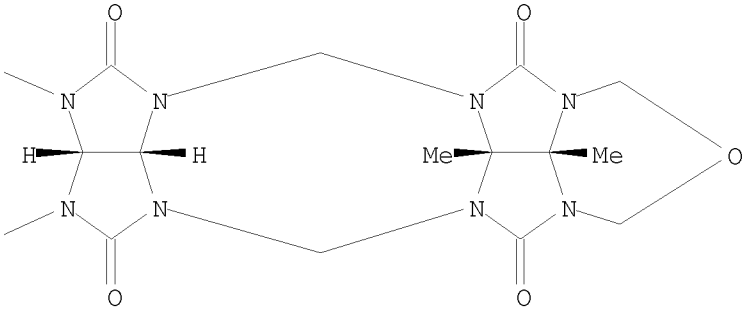
CN 1H,3H,4H,5H,6H,7H,8H,9H,10H,11H,13H,14H,15H,16H,17H,18H,19H,20H-2,12-Dioxa-3a,4a,5a,6a,7a,8a,9a,10a,13a,14a,15a,16a,17a,18a,19a,20a-hexadecaazabisbenzo[3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-4,6,8,10,14,16,18,20-octone, octahydro-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 26 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:260070 CAPLUS
DOCUMENT NUMBER: 142:336358
TITLE: Method for preparing cucurbiturils
INVENTOR(S): Day, Anthony Ivan; Arnold, Alan Peter; Blanch, Rodney John
PATENT ASSIGNEE(S): Unisearch Limited, Australia
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005026168	A1	20050324	WO 2004-AU1232	20040910

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,

AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2004272121	A1	20050324	AU 2004-272121		20040910
CA 2537843	A1	20050324	CA 2004-2537843		20040910
EP 1668012	A1	20060614	EP 2004-761268		20040910
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK					
CN 1878774	A	20061213	CN 2004-80033392		20040910
JP 2007505046	T	20070308	JP 2006-525577		20040910
KR 2006119979	A	20061124	KR 2006-705066		20060311
US 20070066818	A1	20070322	US 2006-571707		20060313
US 7501523	B2	20090310			
IN 2006DN01397	A	20070803	IN 2006-DN1397		20060314
PRIORITY APPLN. INFO.:			AU 2003-905037	A	20030912
			WO 2004-AU1232	W	20040910

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): CASREACT 142:336358; MARPAT 142:336358

AB The invention relates to a method for preparing cucurbiturils. The method comprises reacting an oligomer consisting of 2 to 11 linked glycolurils or glycoluril analogs with one or more compds. selected from glycoluril, glycoluril analogs and/or oligomers of glycoluril or glycoluril analogs, in the presence of an acid, to form a cucurbituril. The method can be used to prepare variably substituted cucurbiturils having specific substituted units at specific locations in the cucurbituril. Thus, dimethylcucurbit[1,4]uril was obtained by treating the formaldehyde diether of dimethylglycoluril with the diether of glycoluril and paraformaldehyde in concentrated HCl.

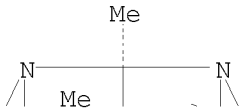
IT 569359-77-9P 848440-55-1P 848440-56-2P
848440-58-4P 848440-61-9P 865813-91-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of cucurbiturils as complexing agents)

RN 569359-77-9 CAPLUS

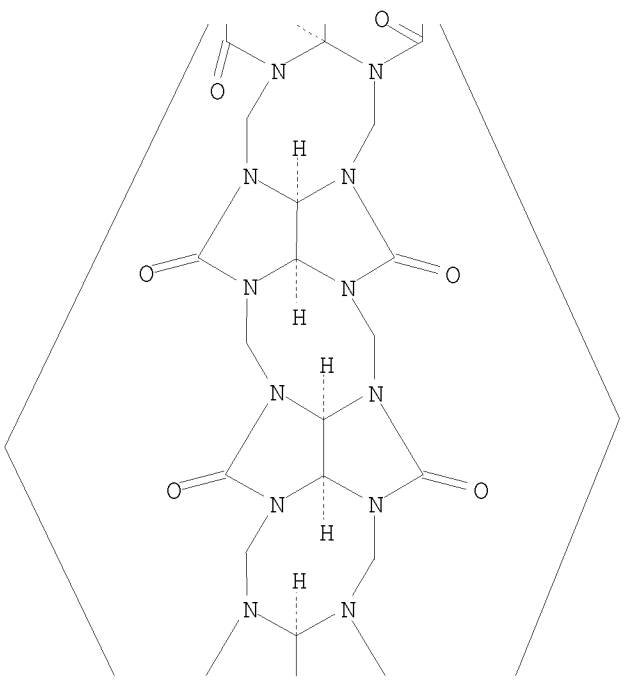
CN 1H,4H,12H,15H-2,14:3,13-Dimethano-
5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pe
ntaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,22b-dimethyl-, stereoisomer
(CA INDEX NAME)

Relative stereochemistry.

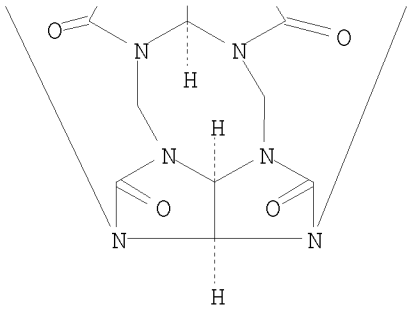
PAGE 1-A



PAGE 2-A

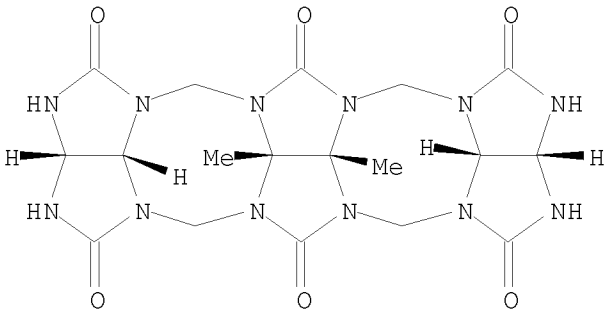


PAGE 3-A



RN 848440-55-1 CAPLUS
CN 5H,6H,7H,12H,13H,14H-2,3,4a,5a,6a,7a,9,10,11a,12a,13a,14a-Dodecaazabispentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,11,13(2H,3H,9H,10H)-hexone, hexahydro-13b,13c-dimethyl-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

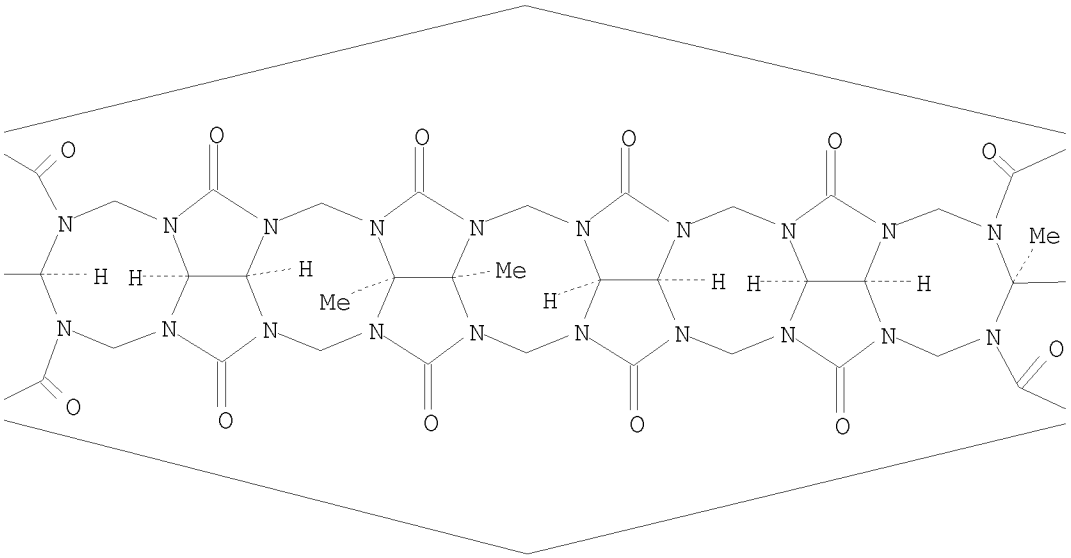


RN 848440-56-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

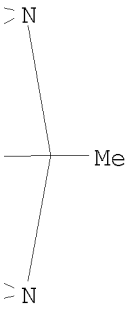
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C

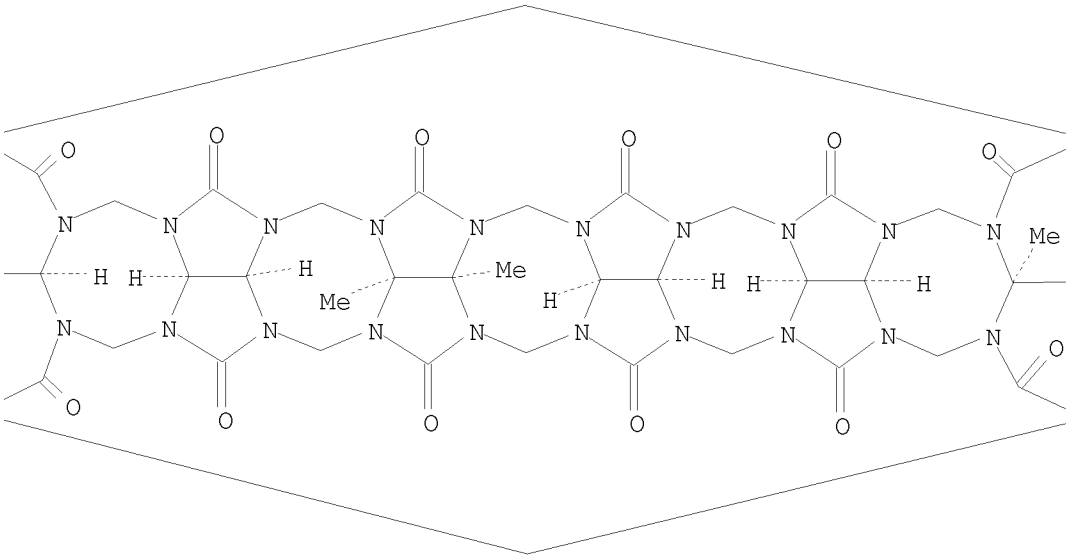


RN 848440-58-4 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24
a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2''
,3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-
g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c-trimethyl-26b-phenyl-, stereoisomer (9CI) (CA
INDEX NAME)

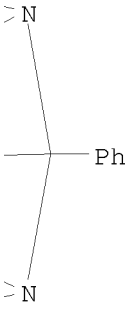
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C

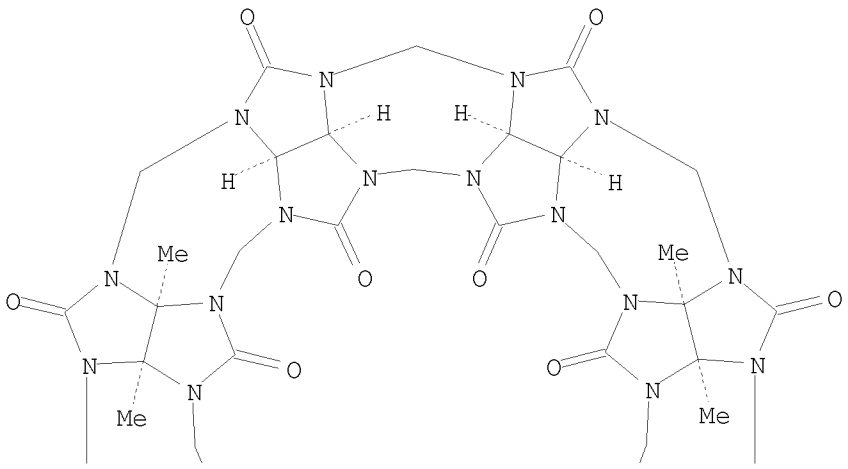


RN 848440-61-9 CAPLUS

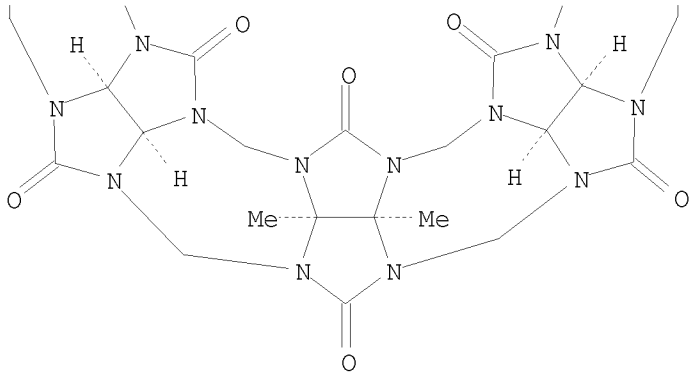
CN 2,18:3,17-Dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,17,18,19a,20a,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a-octacosaazabispentaleno[1''''',6''''':5'''',6'''',7'''']cycloocta[1'''',2''''',3'''':3''',4''']pentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,10,12,14,16,19,21,23,25,27,29-tetradecone, tetradecahydro-2a,21b,21c,25b,25c,30b-hexamethyl-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



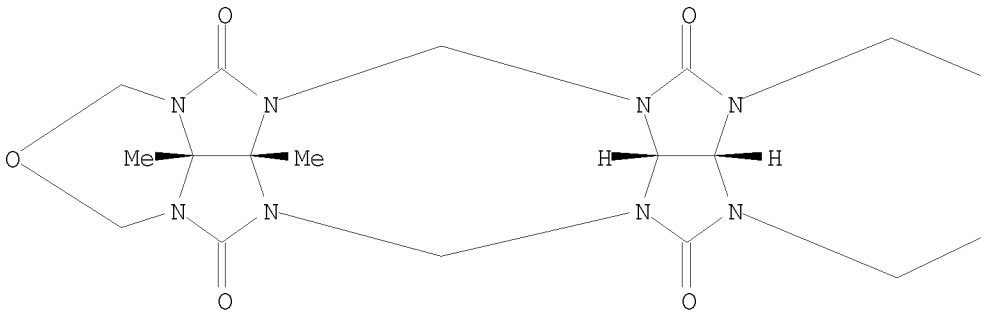
PAGE 2-A



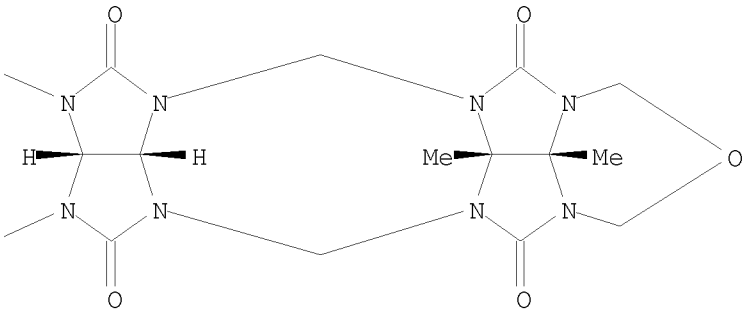
RN 865813-91-8 CAPLUS
CN 1H,3H,4H,5H,6H,7H,8H,9H,10H,11H,13H,14H,15H,16H,17H,18H,19H,20H-2,12-Dioxa-3a,4a,5a,6a,7a,8a,9a,10a,13a,14a,15a,16a,17a,18a,19a,20a-hexadecaazabisbenzo[3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-4,6,8,10,14,16,18,20-octone, octahydro-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 27 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2004:684964 CAPLUS
DOCUMENT NUMBER: 143:7687
TITLE: Synthesis of a symmetrical tetrasubstituted cucurbit[6]uril and its host-guest inclusion complex with 2,2'-bipyridine
AUTHOR(S): Zhao, Yunjie; Xue, Saifeng; Zhu, Qianjiang; Tao, Zhu; Zhang, Jianxin; Wei, Zhanbin; Long, Lasheng; Hu, Maolin; Xiao, Hongping; Day, Anthony I.
CORPORATE SOURCE: Institute of Applied Chemistry, Guizhou University, Guiyang, 550025, Peop. Rep. China
SOURCE: Chinese Science Bulletin (2004), 49(11), 1111-1116
CODEN: CSBUEF; ISSN: 1001-6538
PUBLISHER: Science in China Press
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:7687
AB Synthesis of a sym. tetramethylcucurbit[6]uril (TMeQ[6]) has been achieved by using the diether of dimethylglycoluril and the dimer of glycoluril. The structure of TMeQ[6] has been determined by single crystal X-ray diffraction, 1H NMR spectroscopy and ESMS. The 1H NMR spectra of 2,2'-bipyridine added to TMeQ[6] reveal that the host-guest inclusion

complex was easily formed.

IT 848440-56-2P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation and crystal structure of sym. tetrasubstituted cucurbit[6]uril and its host-guest inclusion complex with bipyridine)

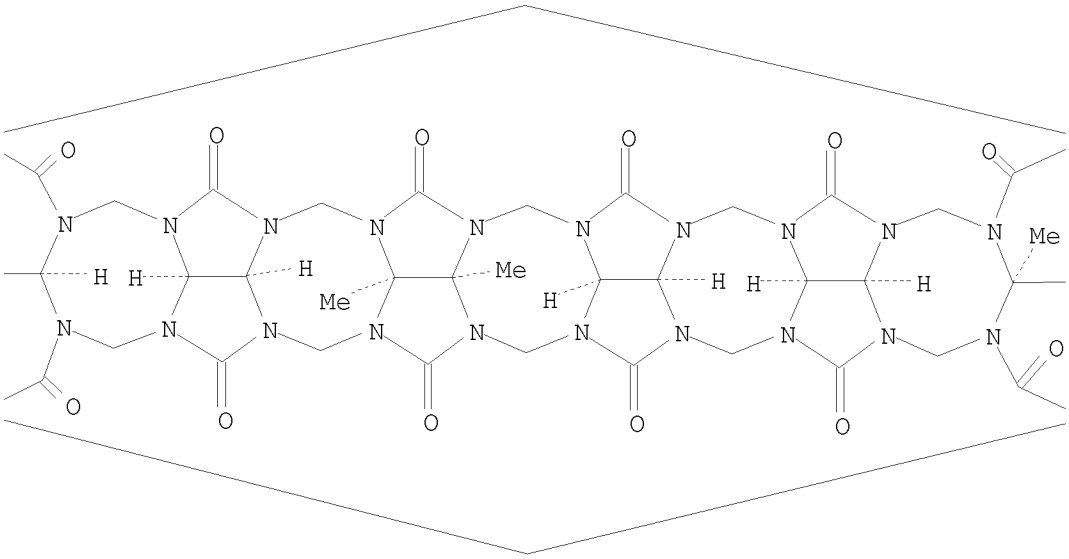
RN 848440-56-2 CAPLUS

CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

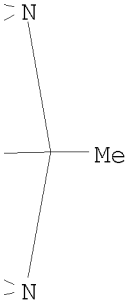
Relative stereochemistry.

PAGE 1-A

PAGE 1-B



PAGE 1-C



OS.CITING REF COUNT: 43 THERE ARE 43 CAPLUS RECORDS THAT CITE THIS RECORD (43 CITINGS)
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 28 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2003:590408 CAPLUS
DOCUMENT NUMBER: 139:135453
TITLE: Cucurbiturils and method for binding gases and volatiles using cucurbiturils
INVENTOR(S): Day, Anthony Ivan; Arnold, Alan Peter; Blanch, Rodney

John
PATENT ASSIGNEE(S): Unisearch Limited, Australia
SOURCE: U.S. Pat. Appl. Publ., 12 pp., Cont.-in-part of U. S. Ser. No. 999,770.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20030140787	A1	20030731	US 2002-301874	20021122
US 6869466	B2	20050322		
WO 2000068232	A1	20001116	WO 2000-AU412	20000505
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6793839	B1	20040921	US 2002-959770	20020107
AU 2002302117	A1	20030320	AU 2002-302117	20021122
AU 2002302117	B2	20060810		
IN 2006DE02152	A	20070907	IN 2006-DE2152	20060928

PRIORITY APPLN. INFO.:			
AU 1999-232	A	19990507	
WO 2000-AU412	W	20000505	
AU 2001-9031	A	20011122	
US 2002-959770	A2	20020107	
AU 2000-43851	A	20000505	
IN 2000-DE485	A3	20000508	

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

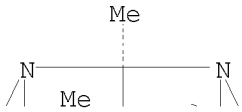
AB Gases or volatile compds. are bound by cucurbiturils as a cucurbituril-gas/volatile complex. The gases or volatile compds. can be separated from a mixture of compds. by contacting the mix with a cucurbituril whereby at least some of the gas or volatile compound is bound to the cucurbituril to form a cucurbituril complex, followed by the release of at least some of the bound gas or volatile compound from that complex. The use of cucurbiturils in binding gases and volatile compds. is suitable for storage, safety, delivery or other uses, such as the trapping of an unpleasant or toxic gas or volatile compound

IT 569359-77-9 569363-90-2 569363-91-3
RL: TEM (Technical or engineered material use); USES (Uses)
(cucurbiturils and method for binding gases and volatiles using cucurbiturils)

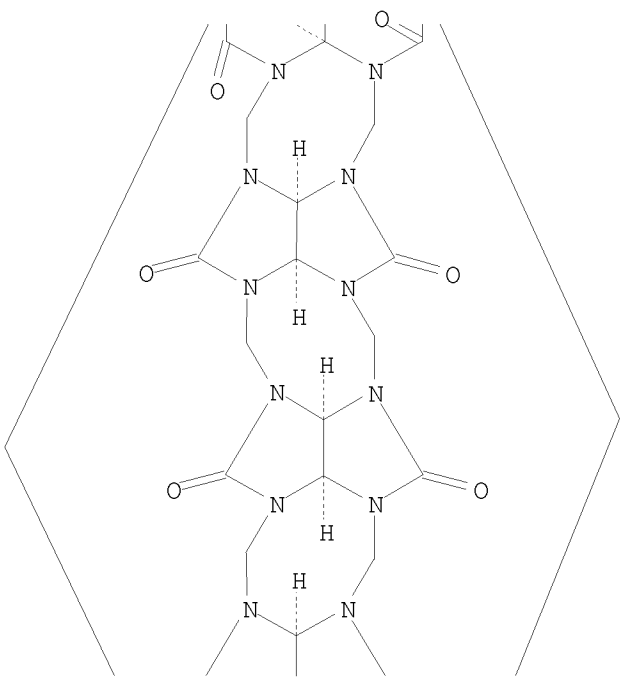
RN 569359-77-9 CAPLUS
CN 1H,4H,12H,15H-2,14:3,13-Dimethano-5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,22b-dimethyl-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

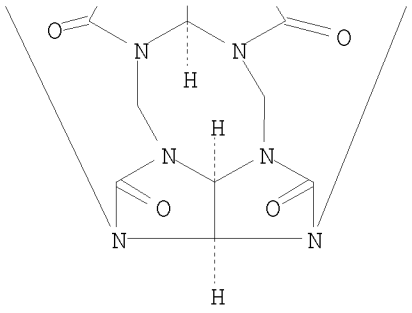
PAGE 1-A



PAGE 2-A

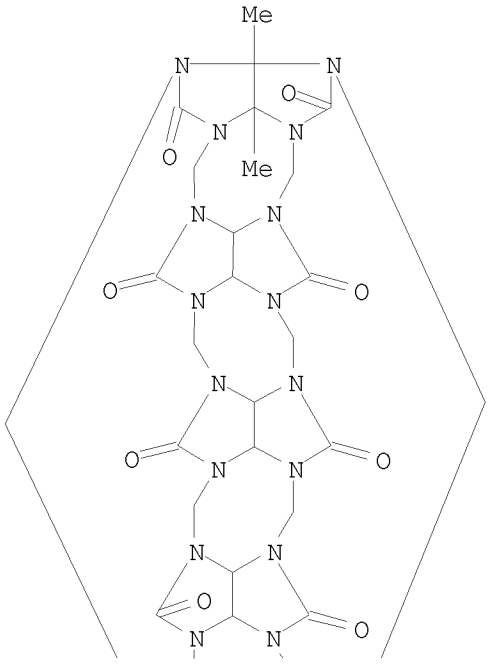


PAGE 3-A

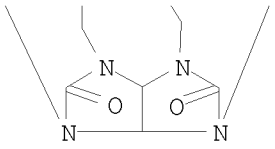


RN 569363-90-2 CAPLUS
CN 1H,4H,12H,15H-2,14:3,13-Dimethano-
5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pe
ntaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,13a,15b,22b(or
2a,17b,17c,22b)-tetramethyl-, stereoisomer (9CI) (CA INDEX NAME)

PAGE 1-A

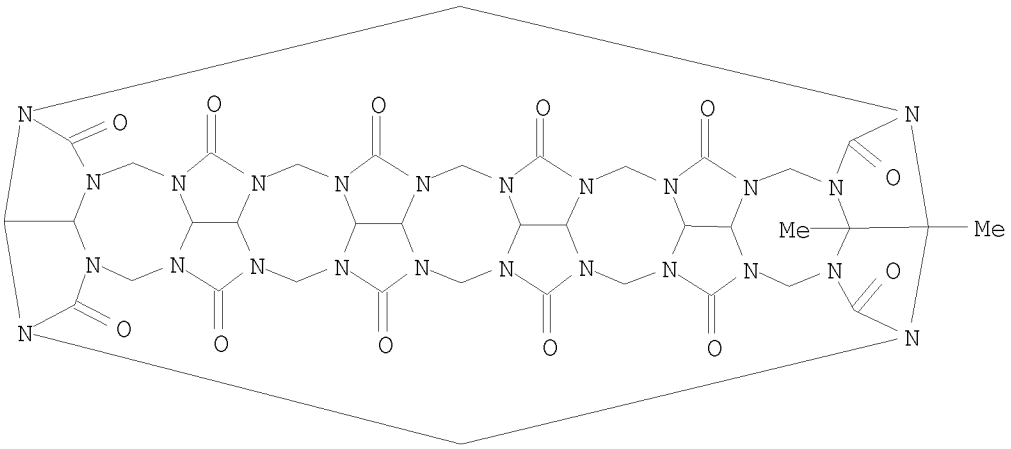


PAGE 2-A



2 (D1—Me)

RN 569363-91-3 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,26b,?,?,?,?-hexamethyl-, stereoisomer (9CI) (CA INDEX NAME)



4 (D1—Me)

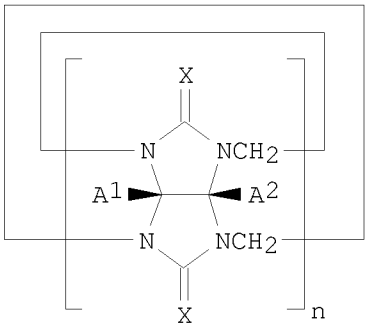
OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

L4 ANSWER 29 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2003:532669 CAPLUS
DOCUMENT NUMBER: 139:101129
TITLE: Methods for preparation of hydroxycucurbituril derivatives and their uses

INVENTOR(S): Kim, Ki-Moon; Jon, Sang-Yong; Selvapalam, Narayanan; Oh, Dong-Hyun
PATENT ASSIGNEE(S): Postech Foundation, S. Korea
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003055888	A1	20030710	WO 2002-KR2213		20021126
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
KR 2003060053	A	20030712	KR 2002-68362		20021106
CA 2468801	A1	20030710	CA 2002-2468801		20021126
AU 2002361511	A1	20030715	AU 2002-361511		20021126
AU 2002361511	B2	20061005			
EP 1463732	A1	20041006	EP 2002-796981		20021126
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK					
CN 1604899	A	20050406	CN 2002-825227		20021126
JP 2005526708	T	20050908	JP 2003-556418		20021126
NZ 533179	A	20060331	NZ 2002-533179		20021126
IN 2004DN01493	A	20070316	IN 2004-DN1493		20040601
US 20050075498	A1	20050407	US 2004-497464		20040602
US 7388099	B2	20080617			
US 20080260676	A1	20081023	US 2008-138883		20080613
PRIORITY APPLN. INFO.:			KR 2002-318	A	20020103
			KR 2002-68362	A	20021106
			KR 2002-2002	A	20020103
			WO 2002-KR2213	W	20021126
			US 2004-497464	A3	20040602

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): CASREACT 139:101129; MARPAT 139:101129
GI



I

AB Provided are hydroxycucurbituril derivs., e.g., I [A1, A2 = OH, (un)substituted C1-30-alkoxy, C1-30-alkenyloxy (sic), C1-30-alkynyloxy (sic), C2-30-carbonylalkoxy, C1-30-thioalkoxy, C1-30-alkylthioloxy, C1-30-hydroxyalkoxy, C1-30-alkylsilyloxy, C1-30-aminoalkoxy, C1-30-aminoalkylthioalkoxy, C5-30-cycloalkoxy, C2-30-heterocycloalkoxy, C6-30-aryloxy, C6-20-arylalkoxy, C4-30-heteroaryloxy , C1-30-alkylthio, C1-30-alkenylthio (sic), C1-30-alkynylthio (sic), C2-30-carbonylalkylthio, C1-30-alkylsilylthio, C1-30-aminoalkylthio, C1-30-aminoalkylthioalkylthio, C5-30-cycloalkylthio, C2-30-heterocycloalkylthio, C6-30-arylthio, C6-20-arylalkylthio (sic), C4-30-heteroarylthio, C4-30-heteroarylalkylthio, C1-30-alkylamino, C1-30-alkenylamino (sic), C1-30-alkynylamino (sic), C2-30-carbonylalkylamino, C1-30-thioalkylamino, C1-30-hydroxyalkylamino, C1-30-alkylsilylamino, C1-30-aminoalkylamino, C5-30-cycloalkylamino, C2-30-heterocycloalkylamino, C6-30-arylamino, C4-30-heteroarylamino; A1 = A2 = H; X = O, S, NH; n = 4 - 20], their preparation methods and uses. Thus, hydroxycucurbit[6]uril (I; A1 = A2 = OH, X = O, n = 6) was prepared in 55% yield from cucurbit[6]uril (I; A1 = A2 = H, X = O, n = 6) via oxidation with aqueous K2S2O8. The hydroxycucurbituril derivative is easy to further functionalize with enhanced solubility in common solvents, thereby providing wider applications, e.g., in agrochems., cosmetics, medicinals and wastewater treatment. Hydroxycucurbit[6]uril formed: a 1:1 host-guest complex with THF; a 1:1 host-guest complex with isobutene; and formed an ion selective membrane with polyvinyl chloride.

IT 558445-98-0P
RL: AMX (Analytical matrix); BSU (Biological study, unclassified); MOA (Modifier or additive use); REM (Removal or disposal); SPN (Synthetic preparation); TEM (Technical or engineered material use); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(preparation of hydroxycucurbituril derivs. and their uses)

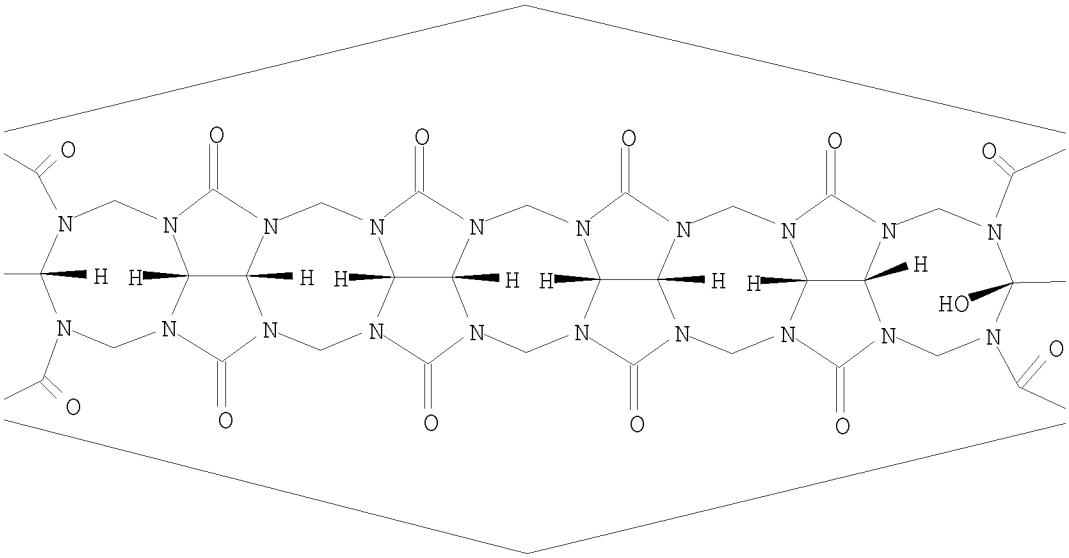
RN 558445-98-0 CAPLUS

CN 1H,4H,14H,17H-2,16:3,15-Dimethano-5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro-2a,26b-dihydroxy-, stereoisomer (9CI) (CA INDEX NAME)

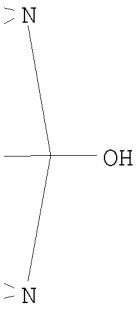
Relative stereochemistry.

PAGE 1-A

PAGE 1-B

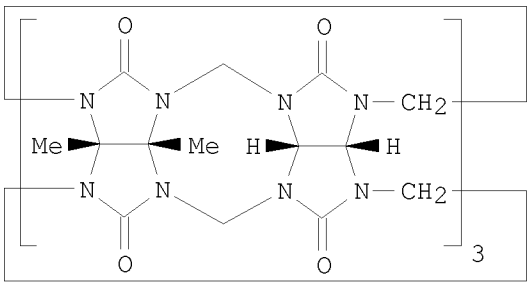


PAGE 1-C



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 30 OF 30 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2003:316145 CAPLUS
DOCUMENT NUMBER: 140:77122
TITLE: A method for synthesizing partially substituted cucurbit[n]uril
AUTHOR(S): Day, Anthony I.; Arnold, Alan P.; Blanch, Rodney J.
CORPORATE SOURCE: School of Chemistry, University College (UNSW), Australian Defence Force Academy, Canberra, ACT 2600, Australia
SOURCE: Molecules (2003), 8(1), 74-84
CODEN: MOLEFW; ISSN: 1420-3049
URL: http://www.mdpi.org/molecules/papers/80100074.pdf
PUBLISHER: Molecular Diversity Preservation International
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:77122
GI



I

AB A novel approach to cucurbituril synthesis is described where partial substitution is introduced into cucurbit[n]uril. The identification of homologs (and their substitution) in reaction mixts. is achieved by a combination of ESMS and the use of the mol. probes (guests) 1,4-dioxane and 1,9-octanediamine. A unique sym. hexamethylcucurbit[3,3]uril (I), the major product, was isolated and characterized.

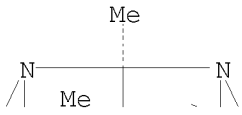
IT 569359-77-9P 640732-36-1P 640732-37-2P
640732-38-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(cyclocondensation of glycouril and its dimethyltetracyclic ether in preparation of partially substituted cucurbituril cyclic oligomers)

RN 569359-77-9 CAPLUS

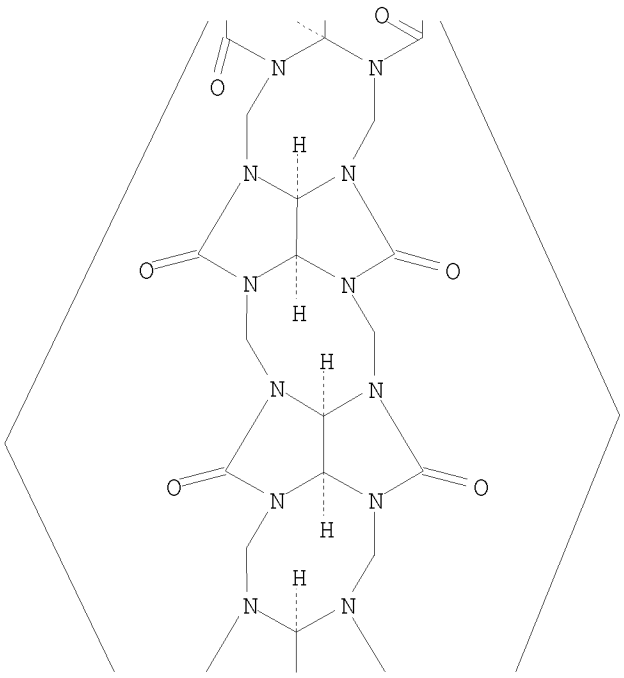
CN 1H,4H,12H,15H-2,14:3,13-Dimethano-
5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,22b-dimethyl-, stereoisomer
(CA INDEX NAME)

Relative stereochemistry.

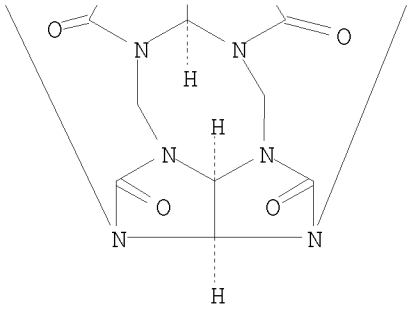
PAGE 1-A



PAGE 2-A



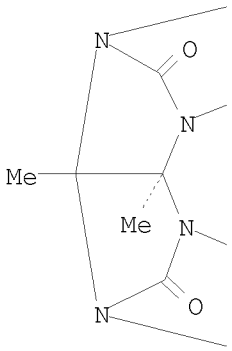
PAGE 3-A



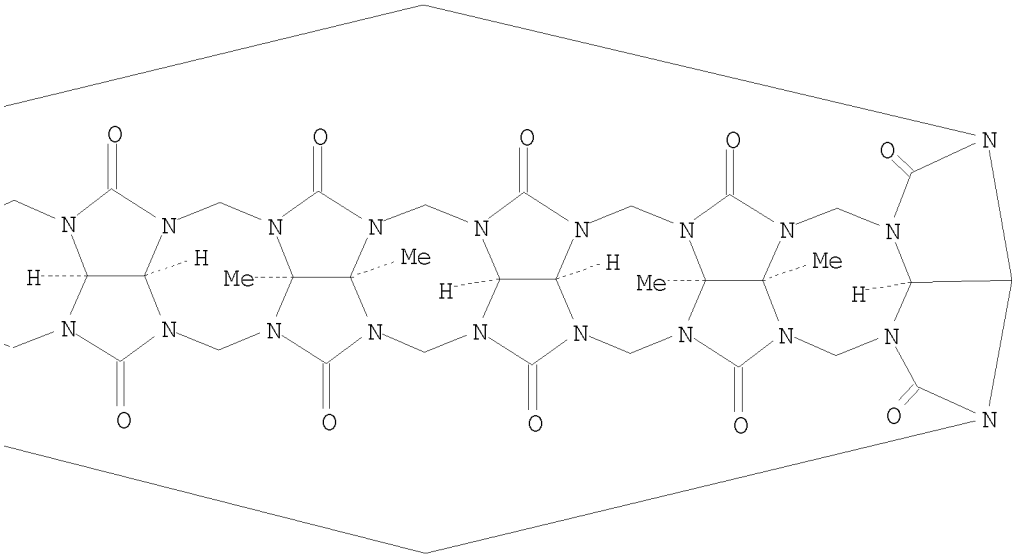
RN 640732-36-1 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,19b,19c,23b,23c,26b-hexamethyl-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



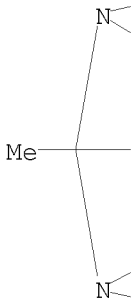
PAGE 1-B



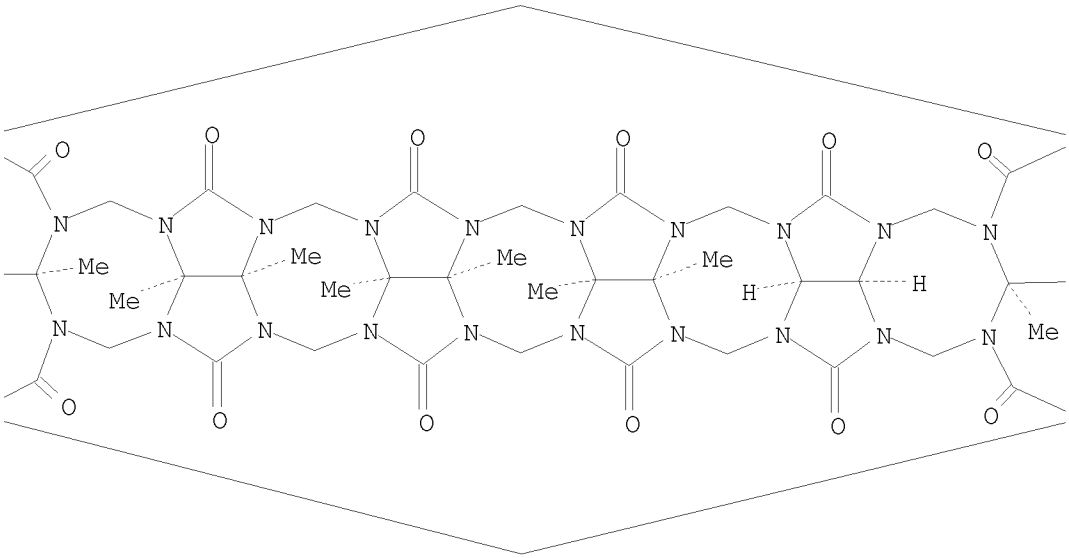
RN 640732-37-2 CAPLUS
CN 1H,4H,14H,17H-2,16:3,15-Dimethano-
5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosaazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
dodecahydro-2a,15a,17b,19b,19c,21b,21c,23b,23c,26b-decamethyl-,
stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

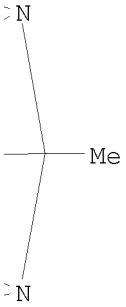
PAGE 1-A



PAGE 1-B



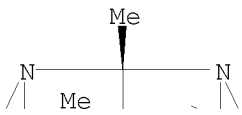
PAGE 1-C



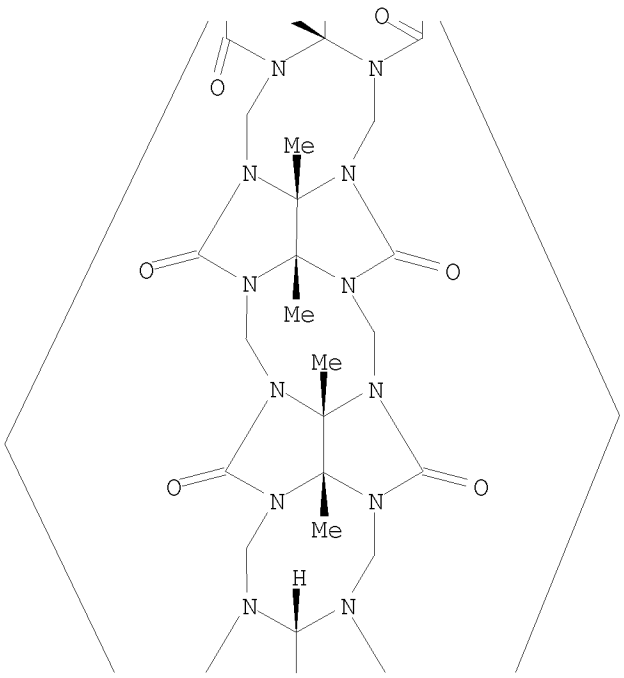
RN 640732-38-3 CAPLUS
CN 1H,4H,12H,15H-2,14:3,13-Dimethano-
5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
eicosaazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pe
ntaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,13a,15b,17b,17c,19b,19c,22b-
octamethyl-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

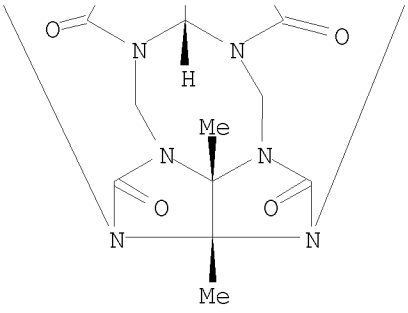
PAGE 1-A



PAGE 2-A



PAGE 3-A



OS.CITING REF COUNT: 47 THERE ARE 47 CAPLUS RECORDS THAT CITE THIS RECORD (47 CITINGS)
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log h

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	174.80	366.56

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-25.50	-25.50

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 21:47:15 ON 28 JAN 2010